



Development and Validation of a Simulation Tool to Predict the Combined Structural, Electrical, Electrochemical, and Thermal Responses of Automotive Batteries

Principal Investigator - Chulheung Bae
Ford Motor Company

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Review and Peer Evaluation Meeting
Jun 12th, 2019

Project ID: BAT296

Overview

Timeline

- Start: Jan 1, 2016
- End: Dec 31, 2019 (with 1-yr no cost extension)
- Percent completion: 80%

Budget

- Total contract value: \$4.375M
 - \$3.5M DOE/TARDEC share
 - \$875k Ford share
- Funding for FY, 2018: \$1.086M
- Funding for FY, 2019: \$1.566M

Barriers Addressed

- Battery/Energy Storage R&D
 - Development Cost
 - Abuse tolerance
 - Robust to the safety requirements

Partners

- Interactions/Collaborations: Oak Ridge National Laboratory (ORNL), Livermore Software Technology Corporation (LSTC), South West Research Institute (SwRI)
- Project Lead: Ford Motor Company

Relevance

- **Project Objective**

- Develop a simulation tool to predict the combined structural, electrical, electrochemical, and thermal (EET) responses of automotive batteries to crash-induced crush and short circuit, overcharge, and thermal ramp and validate it for conditions relevant to automotive crash.
- The failure models will be developed and implemented to be able to further predict response of a deformed batteries after a short circuit occurs.

- **Barriers Addressed**

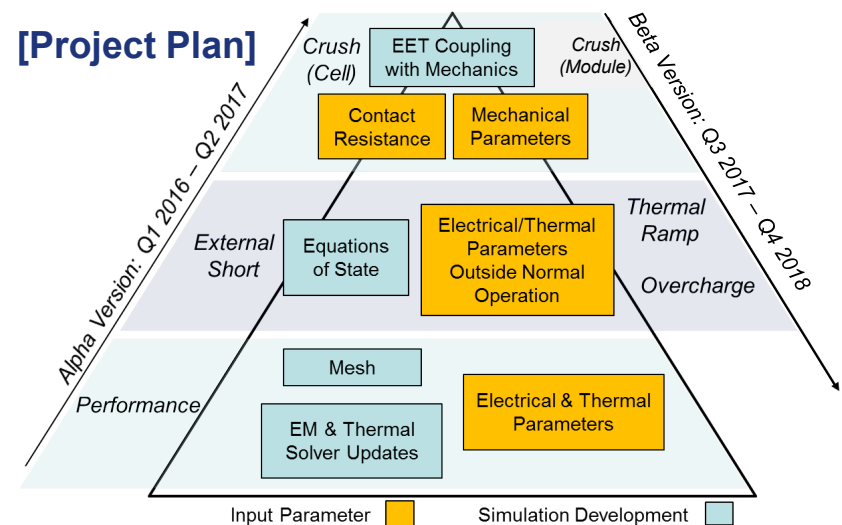
- Cost
 - Cost reduction by shortening development cycle and optimizing crash protection systems.
 - Avoid late-cycle design changes due to regulatory requirement change (i.e. regulatory crush, > 10 s vs. Crash, < 100 ms).
- Abuse tolerance
 - Improvement in abuse tolerance by delivering a predictive simulation tool to shorten or eliminate design – build – test prototype cycles and accelerating development and optimization of crash protection systems robust to the safety requirements.

Milestones

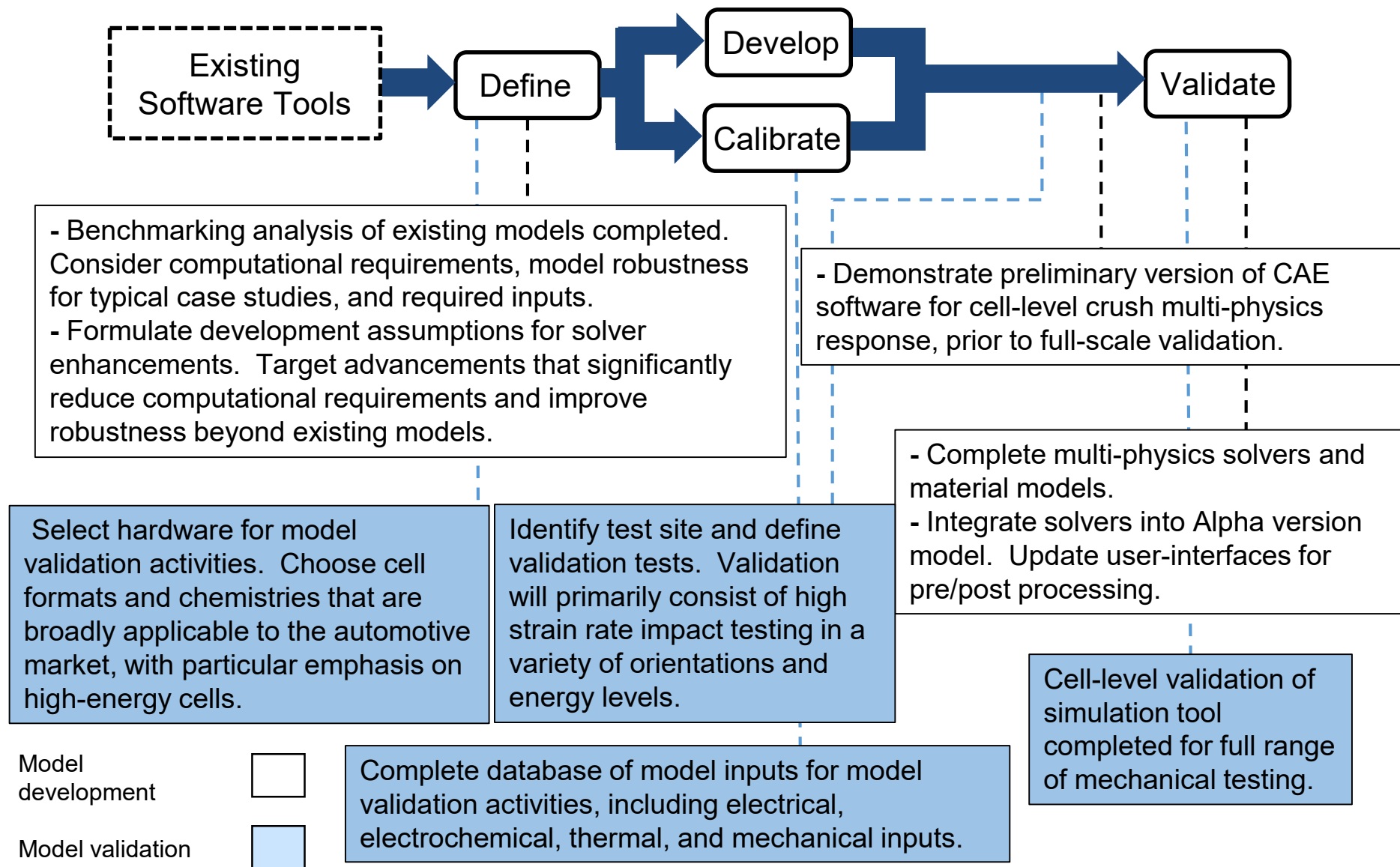
Milestones	2016				2017				2018				2019			
Tasks	Q1	Q2	Q3	Q4	Q1	Q2	Q3	Q4	Q1	Q2	Q3	Q4	Q1	Q2	Q3	Q4
Hardware selection for Alpha version	Complete															
Development assumptions for Alpha version	Complete	Complete														
Alpha version multi-physics solvers and material models		Complete	Complete	Complete	Complete											
Alpha version model inputs		Complete	Complete	Complete	Complete	Complete										
Integrate solvers into Alpha version				Complete	Complete	Complete										
Validation of Alpha version			Behind Schedule (less than 1Q)	Behind Schedule (less than 1Q)	Behind Schedule (less than 1Q)	Behind Schedule (less than 1Q)	Behind Schedule (less than 1Q)	Behind Schedule (less than 1Q)	Behind Schedule (less than 1Q)	Behind Schedule (less than 1Q)	Behind Schedule (less than 1Q)	Behind Schedule (less than 1Q)	Not started			
Hardware selection for Beta version							Complete	Complete	Complete							
Beta version model validation											Behind Schedule (less than 1Q)		Not started	Not started	Not started	Not started
Beta version multi-physics solvers and material models									On-track	On-track	On-track	On-track	Not started	Not started	Not started	Not started
Beta version model inputs									On-track	On-track	On-track	On-track	Not started	Not started	Not started	Not started
Integrate solvers into Beta version									On-track	On-track	On-track	On-track	Not started	Not started	Not started	Not started
Comparative analysis of model and experiments																Not started

Not started 
 On-track 
 Complete 

Behind Schedule (less than 1Q) 
 Behind Schedule (more than 1Q) 



Approach/Strategy – Model Development and Validation



Technical Accomplishments in 2018

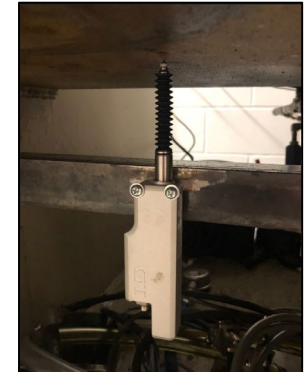
- **Quasi-static cell validation testing was completed for α -version model validation at the previous test supplier, but problems arose and all cell and module testing will now be performed at South West Research Institute (SwRI), where all fixtures and instrumentation are now in place.**
 - 1 yr – no cost extension was requested to rerun the quasi-static tests and complete the high speed impact tests at cell and module levels. It was approved in early Q3, 2018.
 - Preliminary tests were done for fine-tuning the test stands and DAQ systems.
- **X-ray tomography has been used to investigate damage in individual cell layers under shear.**
- **Enhanced the capabilities of the layered solid elements (or composite t-shell elements) in mechanical, electromagnetic (EM), and thermal solvers.**
- **Developed models with layered solid elements under different abuse scenarios and demonstrated its advantages compared with solid element formulations.**
- **New material models were developed treating active materials as granular materials with parameters chosen to yield good results compared to experiments.**
- **Initiated the development of the macro model that aims to improve computational efficiency of the EM and thermal solvers.**

Technical Progress: α and β Version Model Validation Tests

- **Quasi-static test fixture issue**
 - Based on video analyses of the tests, unexpected lateral movement of indenters was observed during the tests leading to irreproducible results.
 - New test company (SwRI) was selected through technical due diligence for the model validation tests.
- **Test setup at SwRI for high speed impact and quasi-static tests**



[High speed impact test stand]

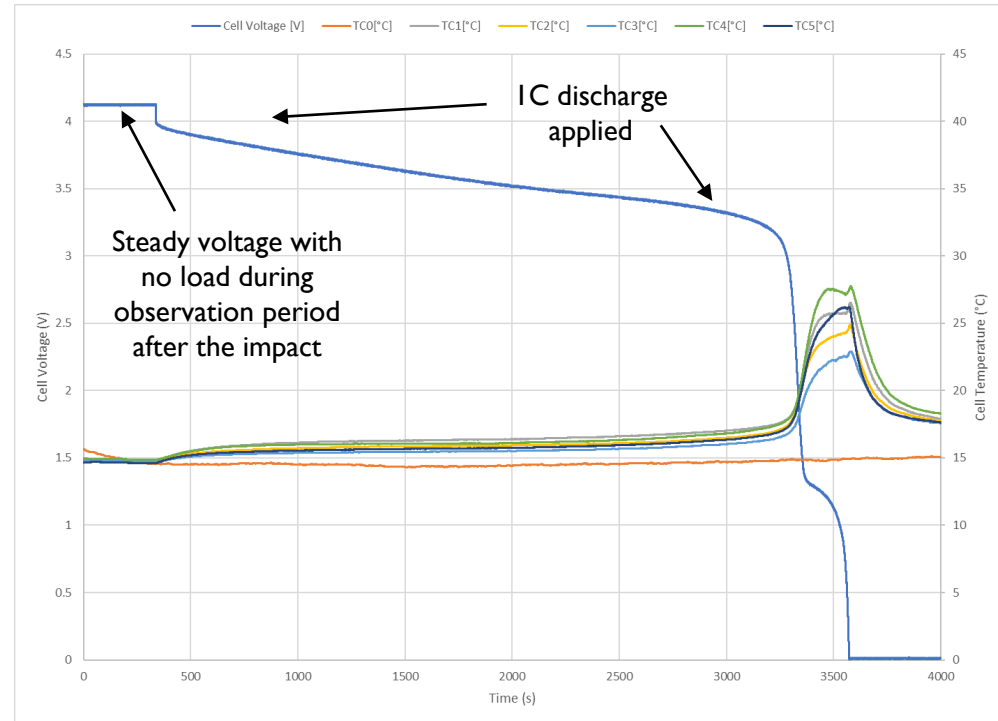
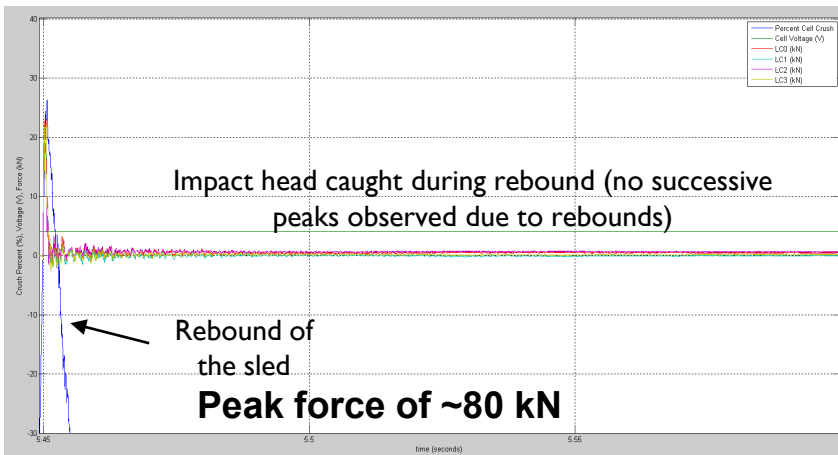
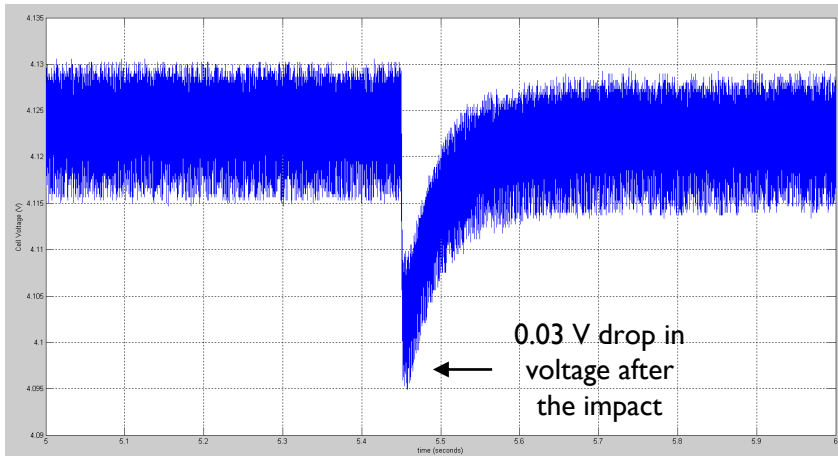


[Quasi-static test stand & LVDT sensor and its location]

Technical Progress: α and β Version Model

Validation Tests Cont'd_Preliminary High Speed Impact Test

- 0.5 m Drop height test with 14.5 kg indenter head



[Voltage and cell body temperature measurements after the impact and during cell discharge to 0V]

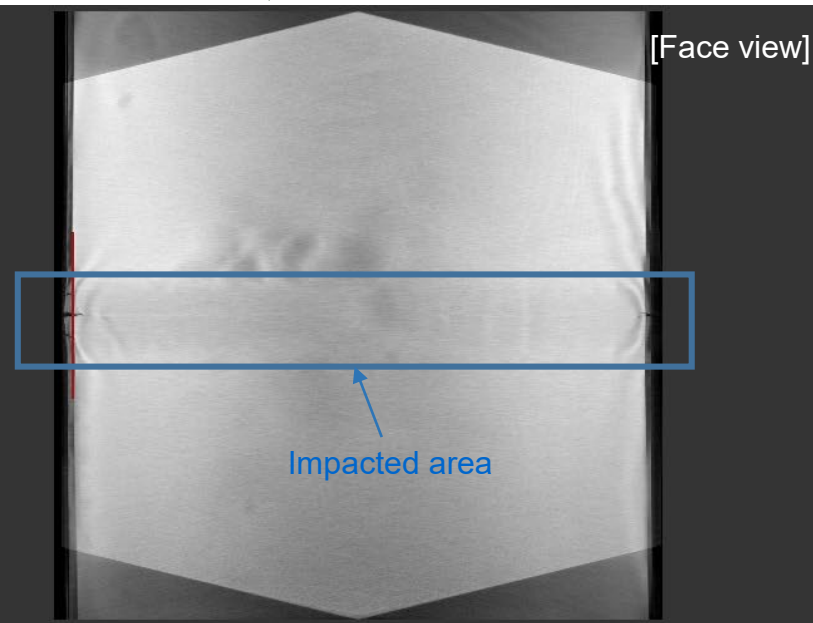
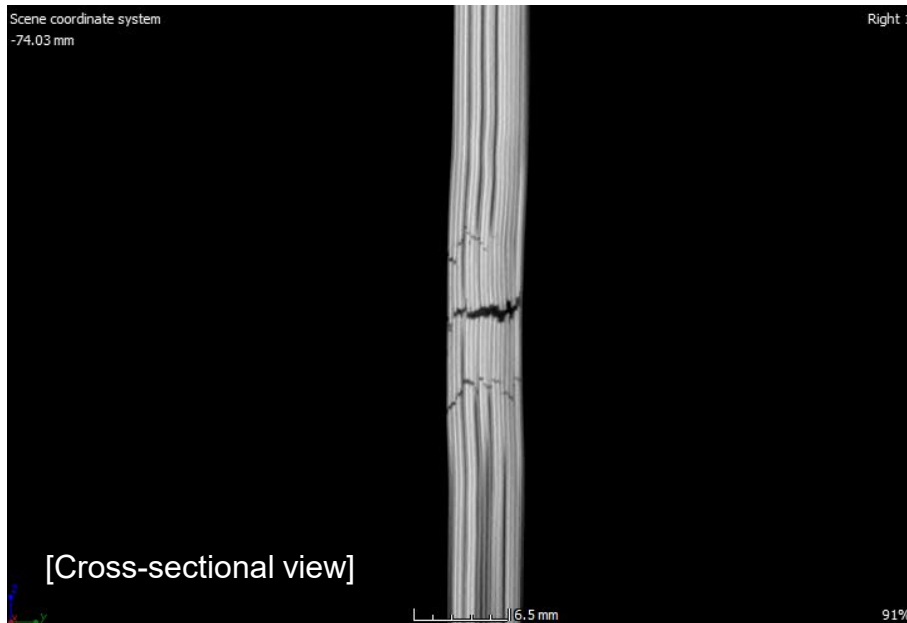
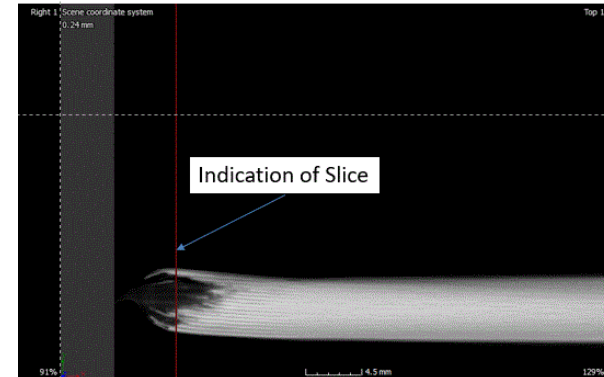
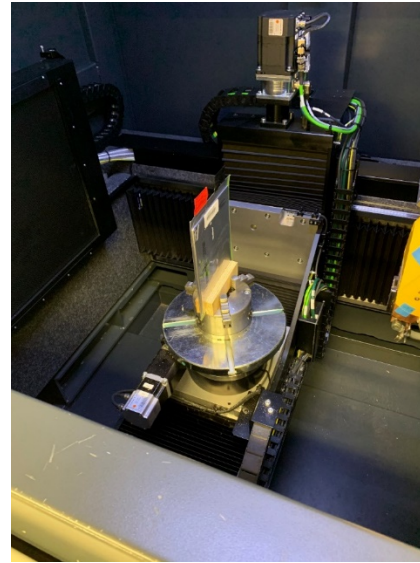
[Voltage and force measurements during high speed impact]

- After observation period, the cell was discharged at 1C to 0V for X-ray CT analysis.

Technical Progress: α and β Version Model

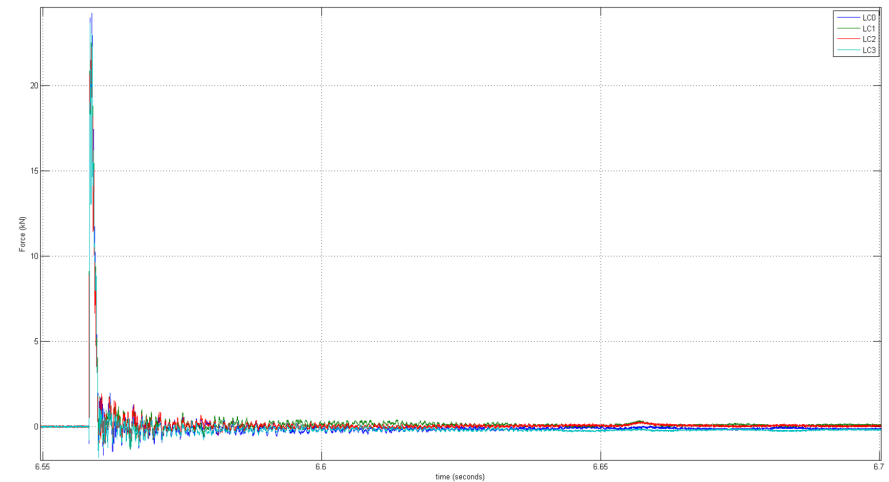
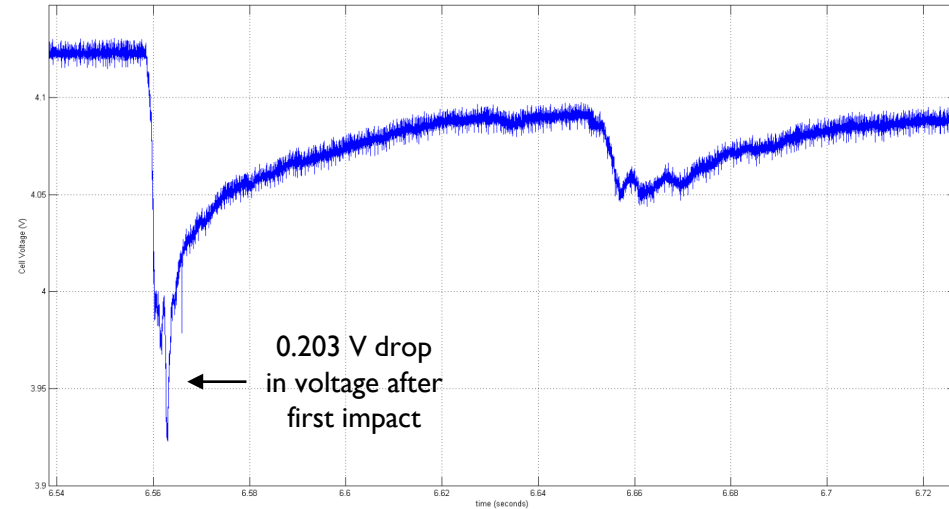
Validation Tests Cont'd_Preliminary High Speed Impact Test

- X-ray Computed Tomography (XCT) analyses of the 0.5 m drop height test cell

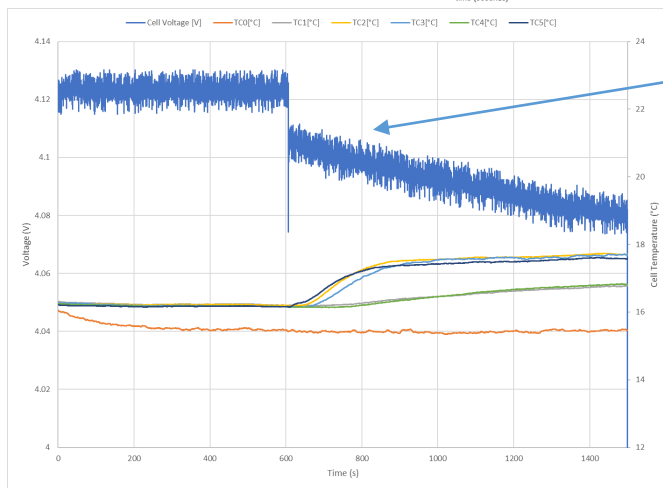


Technical Progress: α and β Version Model Validation Tests Cont'd_Preliminary High Speed Impact Test

- 0.5 m Drop height test with 29 kg indenter head



Peak force of ~100 kN

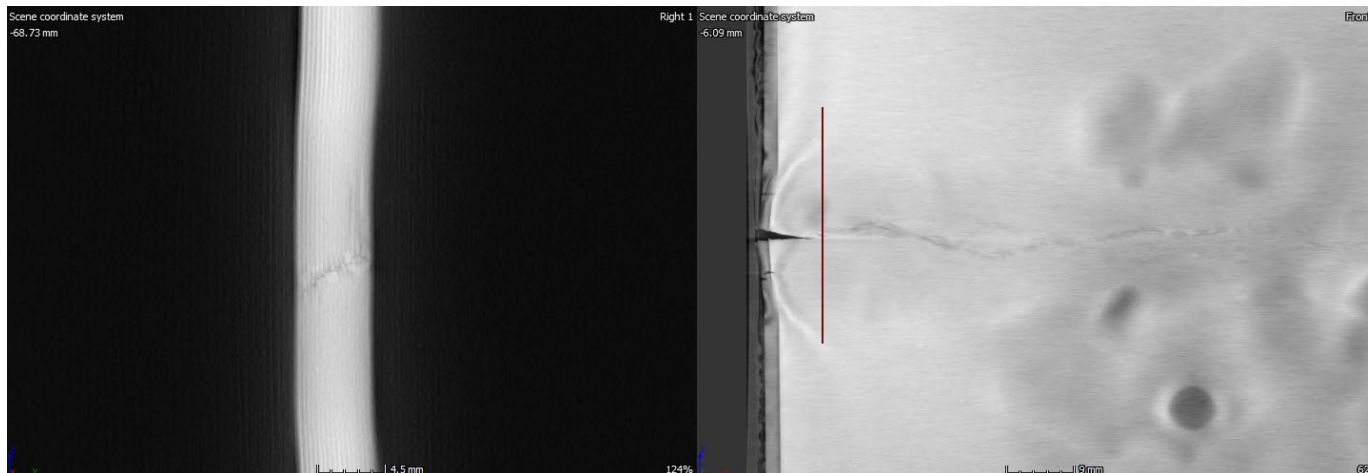
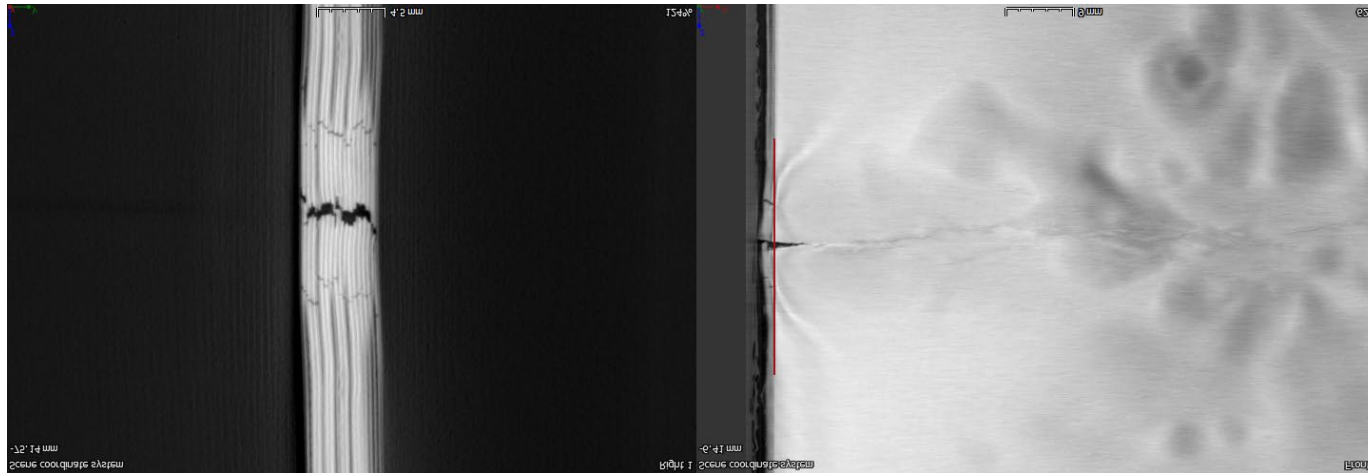


- Cell voltage continued to drop with no load applied after impact: 20 mV in 15 min.

Technical Progress: α and β Version Model

Validation Tests Cont'd_Preliminary High Speed Impact Test

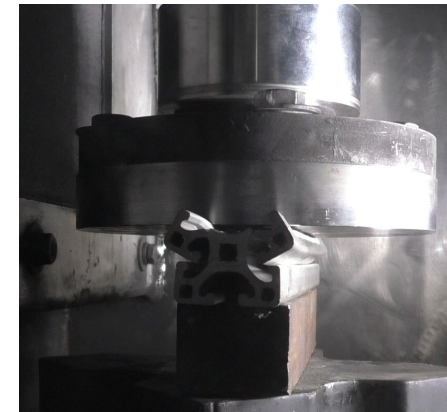
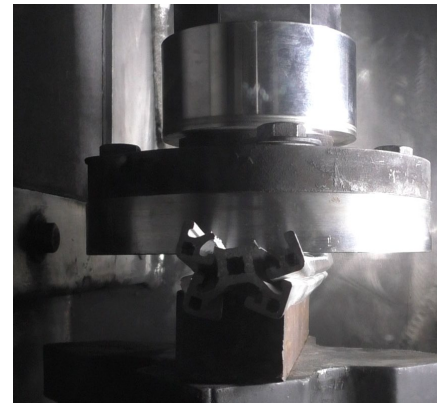
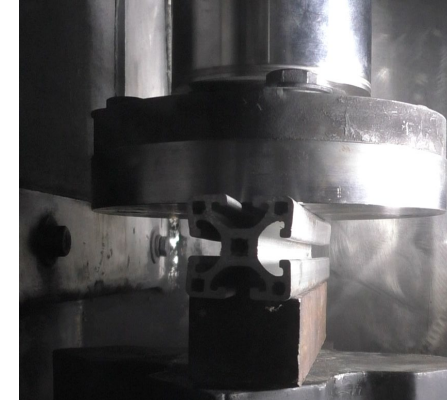
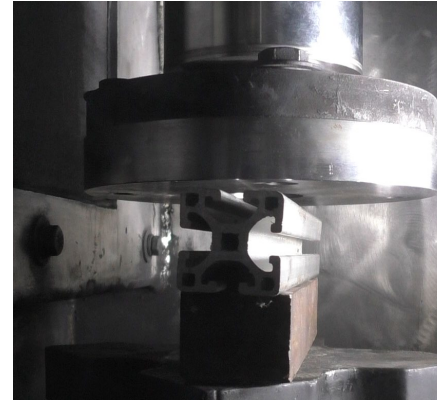
- XCTAnalyses of the 0.5 m drop height test cell (29kg indenter head)



Technical Progress: α and β Version Model

Validation Tests Cont'd_Preliminary Quasi-Static Tests

- **Open loop control**
 - Crushed an aluminum t-slot.
 - Allowed for discontinuities in force when crushing.
- **New hydraulic reservoir installed**

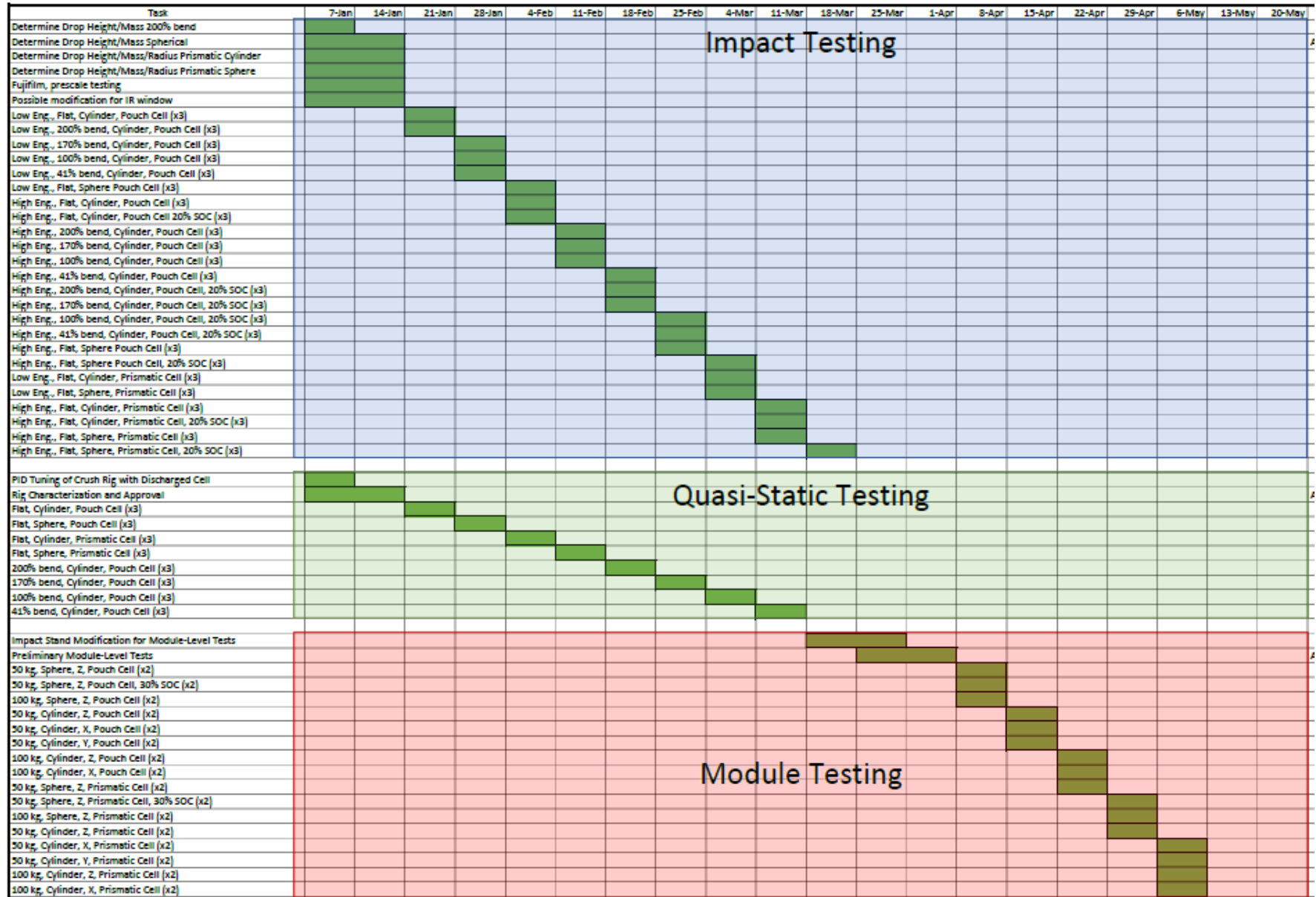


- **Viewing window will be added on the side wall.**

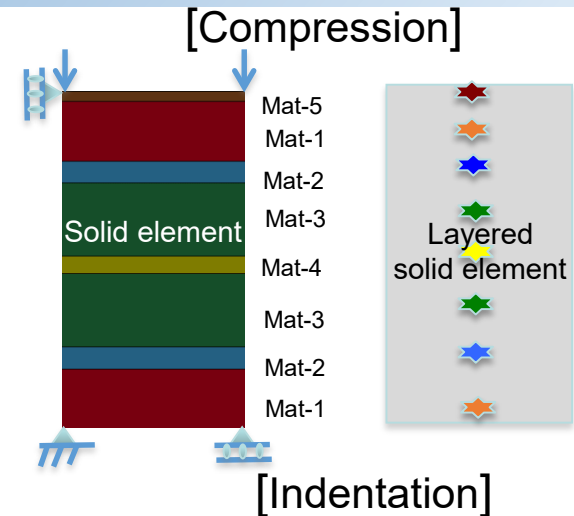
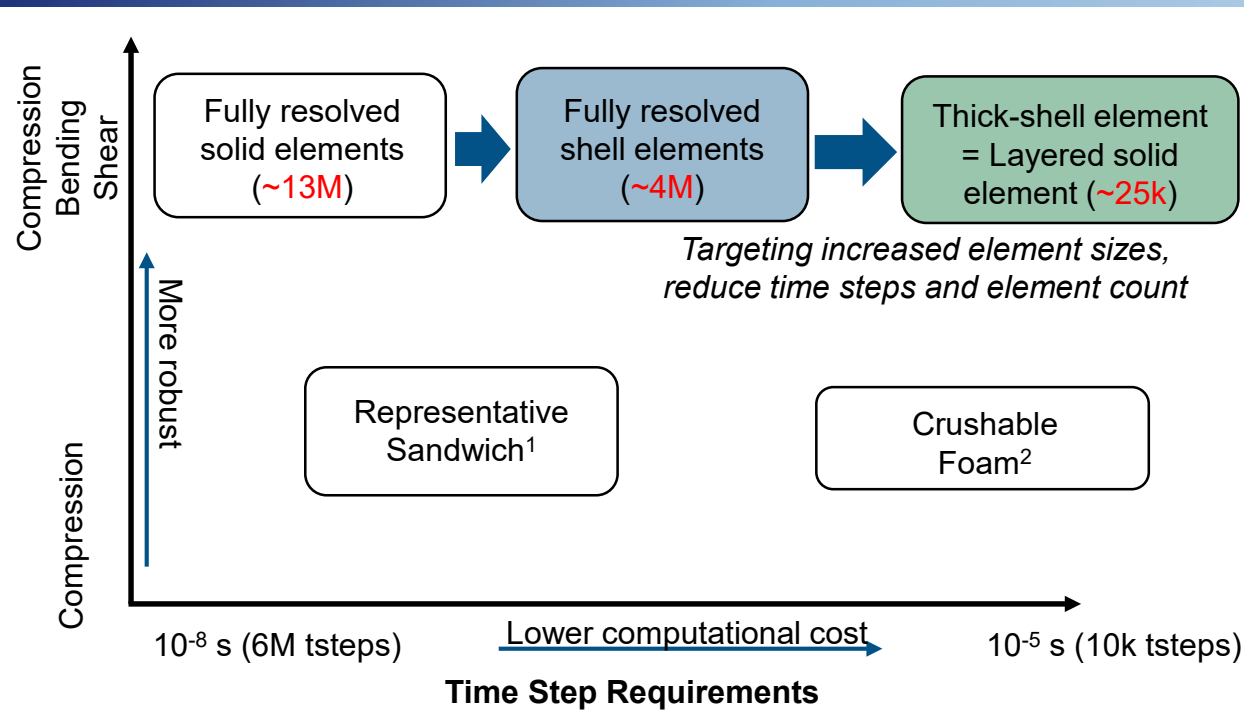
- **Preliminary tests with an aluminum t-slot**

Technical Progress: α and β Version Model

Validation Tests Cont'd_Model Validation Test Schedule



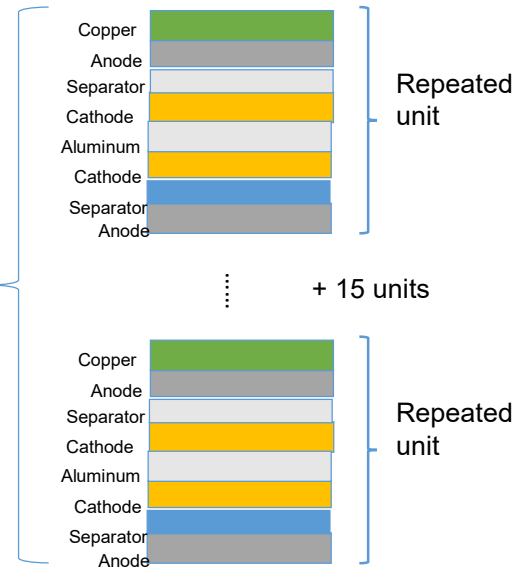
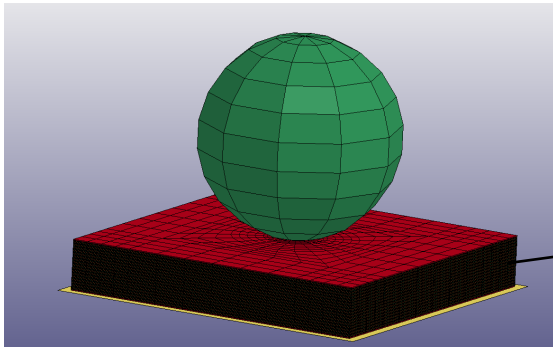
Technical Progress: Development of Layered Solid Element Solver



- Layered solid element solver was developed and verified by comparing its performance against solid element solver's under three deformation modes (compression, indentation, and bending modes)
 - Solid element solver was developed and calibrated using legacy cells' input parameters and empirical data for previous project.
 - Same information was used to verify performance of layered solid element solver against that of proven solid element solver under three different deformation modes.
 - It was observed that the layered solid element provided the same results but much faster computational time compared to solid element (i.e. 105 times faster for indentation).

Technical Progress: Development of Layered Solid Element Solver_Cell Indentation

- **Solid Elements (17 layers resolved)**



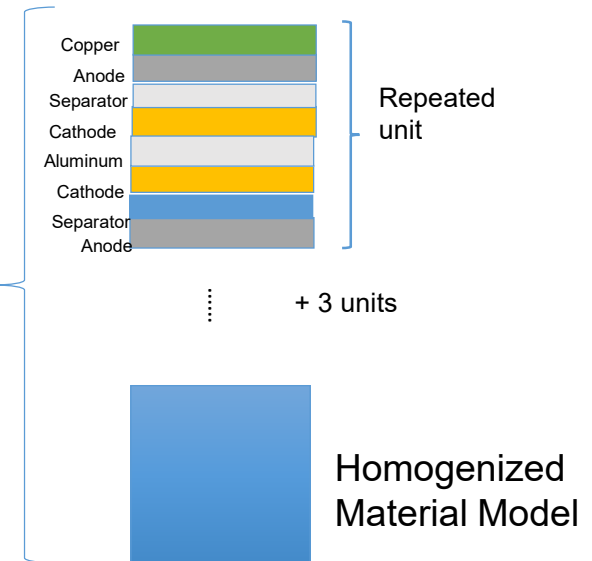
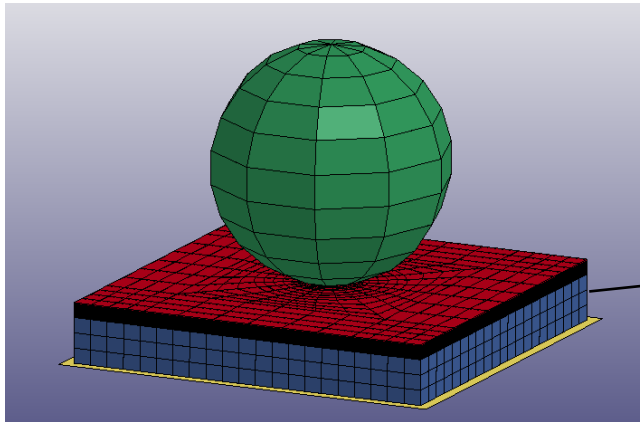
Component	Thickness (mm)	Material Model	Elastic Modulus (GPa)	Yield Strength (GPa)
Copper	0.011	MAT-24	110	0.24
Anode	0.064	MAT-63	0.45	0.04
Separator	0.024	MAT-24	0.5	0.06
Cathode	0.080	MAT-63	0.55	0.04
Aluminum	0.018	MAT-24	70	0.24

- 2 pouch layers at the top and bottom
- 17 total cell layers
- 556 elements per layer
- 76,728 solid elements

- **Gradient mesh was necessary to control the size of the model.**
- **Regular mesh that is the same for the layered element model results in early element inversion and simulation failure.**

Technical Progress: Development of Layered Solid Element Solver_Cell Indentation

- Solid Elements (4 top layers resolved)

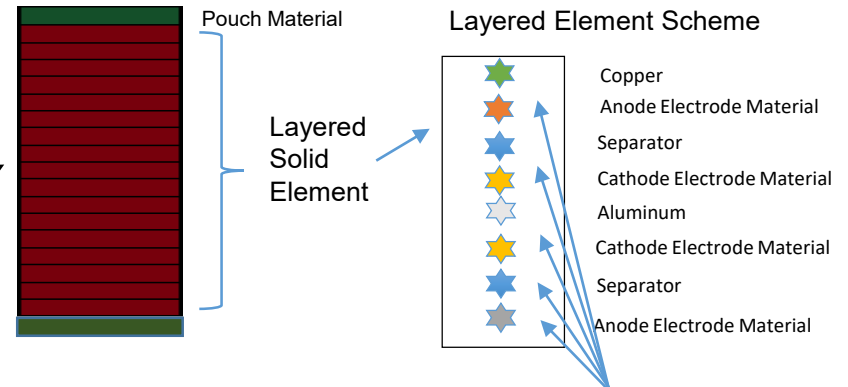
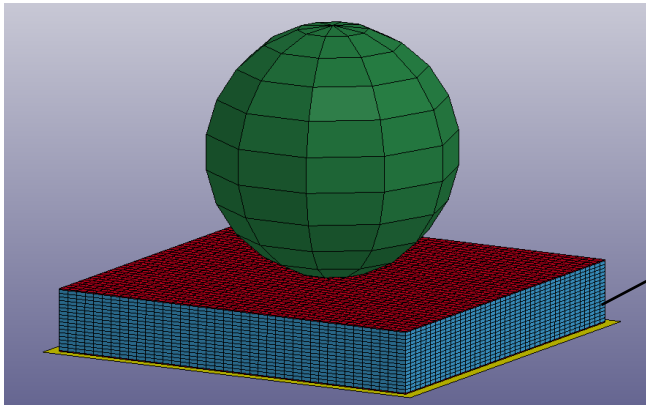


Component	Thickness (mm)	Material Model	Elastic Modulus (GPa)	Yield Strength (GPa)
Copper	0.011	MAT-24	110	0.24
Anode	0.064	MAT-63	0.45	0.04
Separator	0.024	MAT-24	0.5	0.06
Cathode	0.080	MAT-63	0.55	0.04
Aluminum	0.018	MAT-24	70	0.24
Homogenized	3.6	MAT-63	0.50	0.04

- 2 pouch layers at the top and bottom
- 17 total cell layers out of which 4 at the top are resolved
- 556 elements per layer
- 20,227 solid elements

Technical Progress: Development of Layered Solid Element Solver_Cell Indentation

• Layered Solid Elements



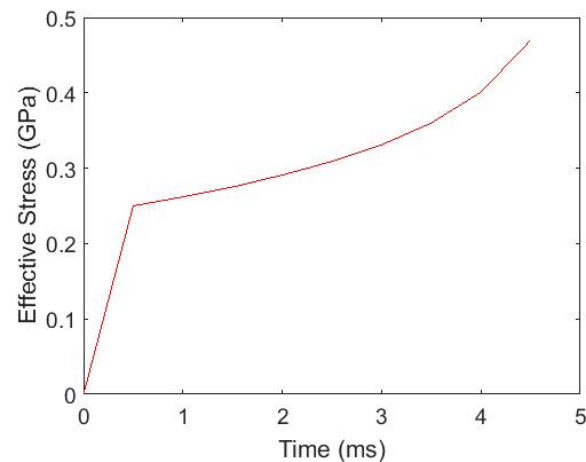
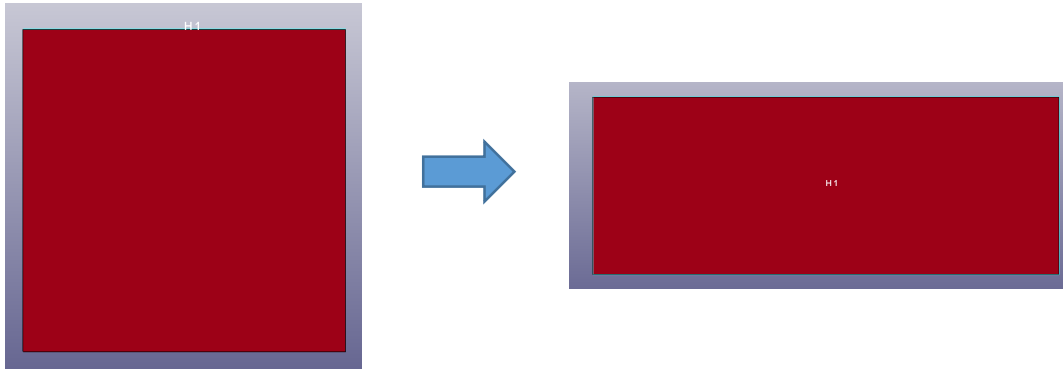
Each jelly-roll component expressed as an integration point in layered solid elements

- 17 total cell layers
- 3,200 solid elements (pouch)
- 27,200 layered solid (cell)
- **Regular Mesh**

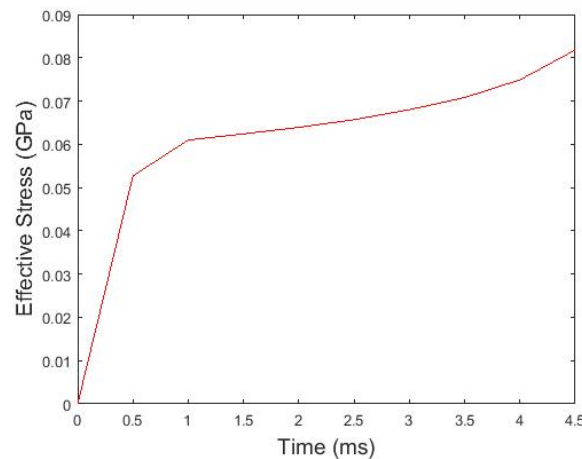
Component	Thickness (mm)	Material Model	Elastic Modulus (GPa)	Yield Strength (GPa)
Copper	0.011	MAT-24	110	0.24
Anode	0.064	MAT-63	0.45	0.04
Separator	0.024	MAT-24	0.5	0.06
Cathode	0.080	MAT-63	0.55	0.04
Aluminum	0.018	MAT-24	70	0.24

Technical Progress: Development of Layered Solid Element Solver_Uniaxial Compression of Single Element

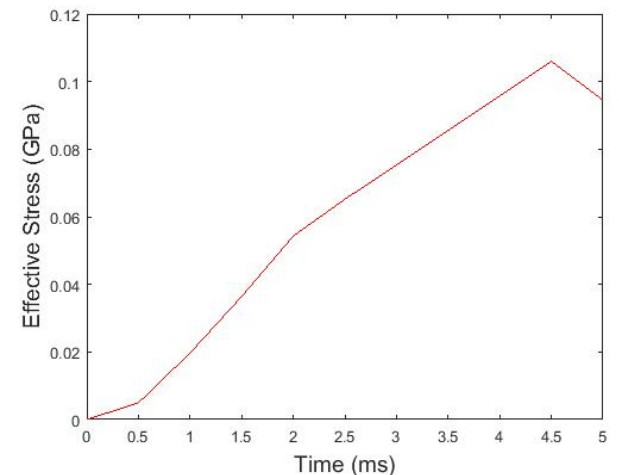
- Compression test of various cell jelly-roll components illustrates expected response.



Stress in Al layer (Mat-24)

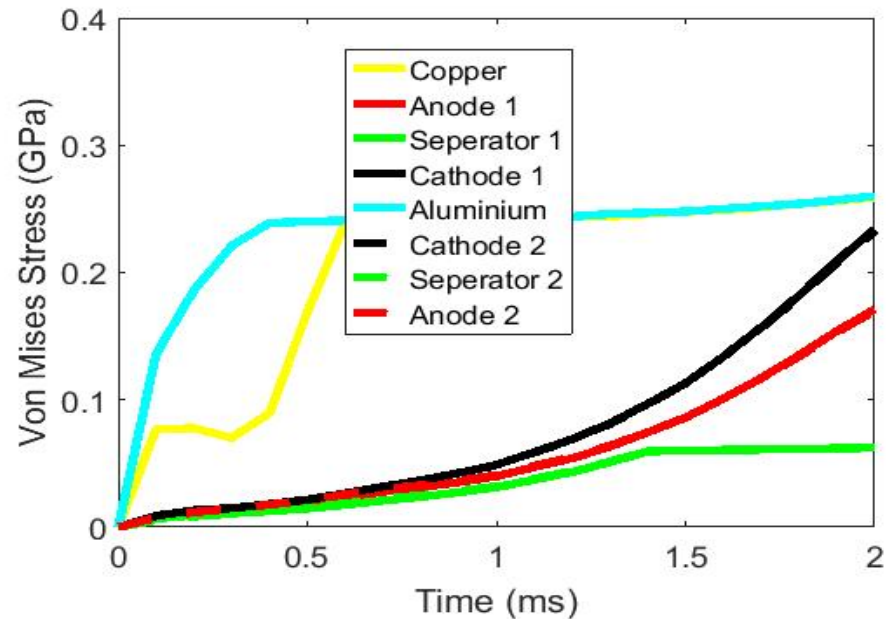
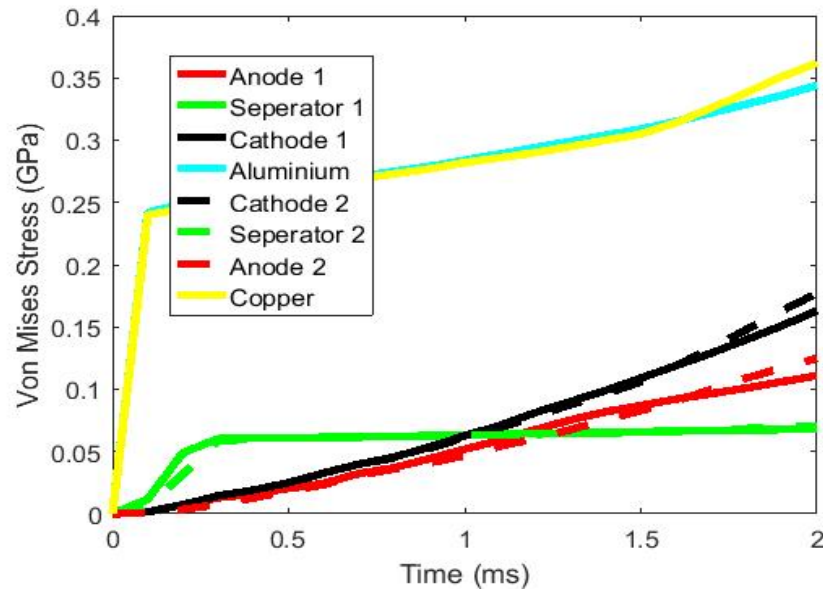


Stress in Separator (Mat-24)

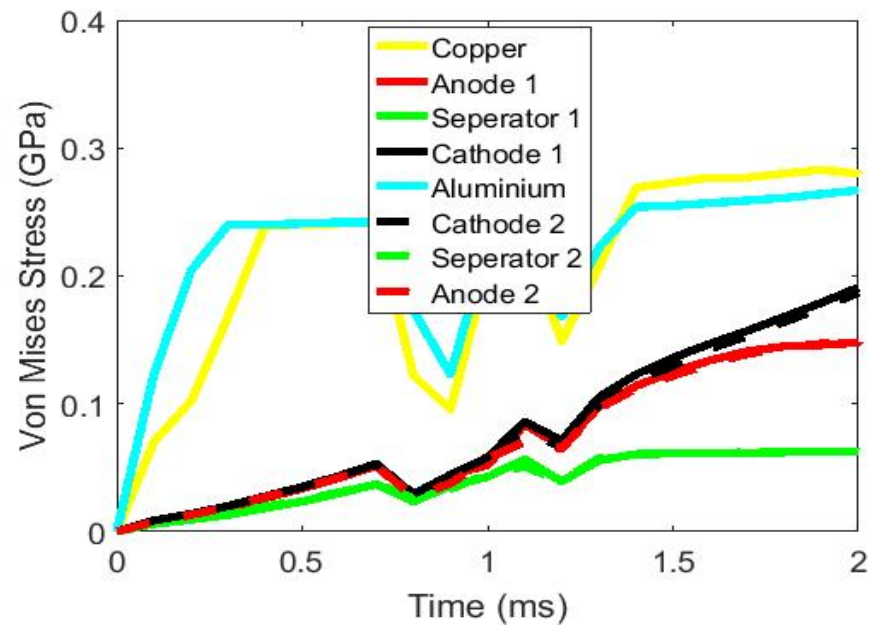


Stress in Anode layer (Mat-63)

Technical Progress: Development of Layered Solid Element Solver_Effective Stress in the Center for Top 8 Components

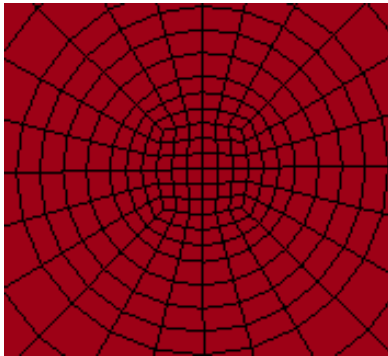


- Separator response in the two models show difference in the early part of deformation. Layered solid model seems to be engaging stretching deformation more quickly than the solid model.
- Solid element model with 17 resolved layers shows oscillations.

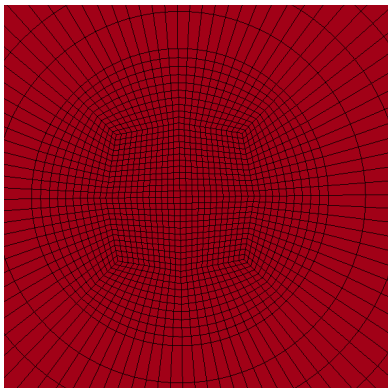


Technical Progress: Development of Layered Solid Element Solver_Effect of the Aspect Ratio for Solid Elements

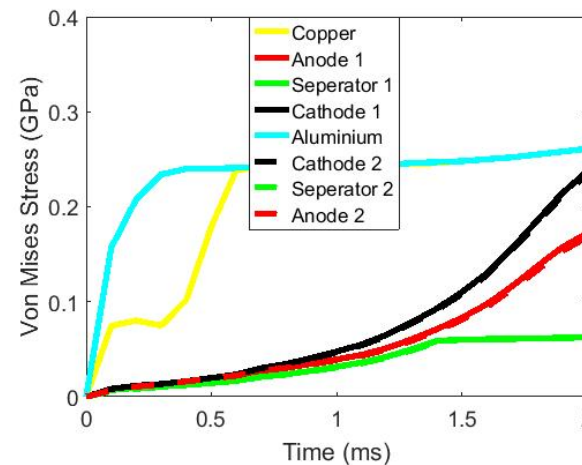
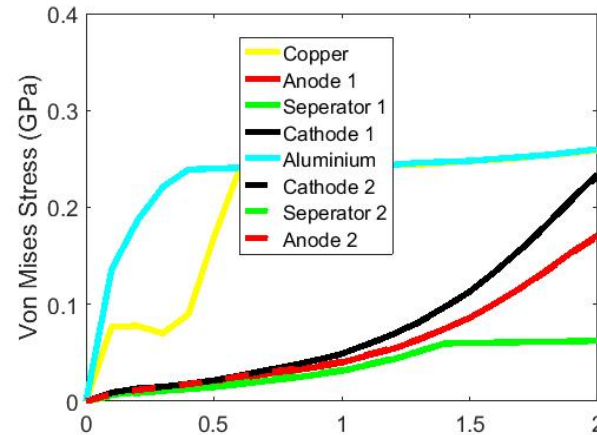
- Solid Elements (4 top layers resolved)



556 element per layer



2896 element per layer



- No difference in stress values after increase in the aspect ratio for the 4 layer resolved solid element model.

Technical Progress: Material Model Development

Constitutive Models for Active Materials

- **Material models for all cell components except for active materials are well established.**
- **Active materials constitute large volume fraction of battery cells.**
- **The active materials have structure of bonded granular materials.**
- **The mechanical response of active materials have been analyzed by X-ray tomography and optical microscopy and was shown to be similar to cohesive granular soils.**
- **Experiments have been conducted and reported in open literature that support the granular solid assumption.**

Technical Progress: Material Model Development

Material Models in LS-DYNA for Granular Materials

- **LS-DYNA has soil and concrete material models.**
- **In the project so far, we used MAT-63 as model for electrode material (crushable foam) but this cannot fully account for the material response and its failure.**
- **In order to model failure of active materials (e.g. crumbling, shear faults) we need to have a material model that allows for failure.**
- **LS-DYNA MAT-145 (Schwer and Murray cap model) is a standard model for modeling soils, rocks concrete, and it has modeling options for modeling degradation and failure.**
 - Large number of parameters.
 - More complicated version of Drucker-Prager model (MAT-193), which does not have failure option.
 - Failure parameters are usually fit to more complex tests and tested for different configurations.
- **In recent publication(*), material model parameters for Drucker-Prager (MAT-193) were reported for anode active material.**
- **We have conducted experiments on anode and cathode materials to determine properties for Drucker-Prager model, as well.**
- **Eventually, we want to use MAT-145 because of its ability to model material damage and failure.**

*J. Zhu et al.; Testing and Modeling the Mechanical Properties of the Granular Materials of Graphite Anode; Journal of The Electrochemical Society (2018).

Technical Progress: Material Model Development

Parameters Transferrable between MAT-193 and MAT-145

- **Comparison of MAT-193 and MAT-145 formulation for basic material model parameters.**

In MAT-193, shear limit surface is defined as

$$t - p \times \tan \beta - d = 0$$

$$t = \sqrt{3J_2} \quad p = \frac{J_1}{3}$$

Limit Stress Equation

$$\sqrt{3J_2} - J_1 \times \frac{\tan \beta}{3} - d = 0$$

$$\sqrt{J_2} - J_1 \times \frac{\tan \beta}{3\sqrt{3}} - \frac{d}{\sqrt{3}} = 0$$

$$\tan \beta = 6 \sin \varphi / (3 - \sin \varphi)$$

$$d = 6C \cos \varphi / (3 - \sin \varphi)$$

In MAT-145, the shear limit surface is defined as

$$\sqrt{J_2} - \alpha + \gamma \exp(-\beta J_1) - \theta J_1 = 0$$

$$\text{For } \gamma = \beta = 0$$

$$\sqrt{J_2} - \alpha - \theta J_1 = 0$$

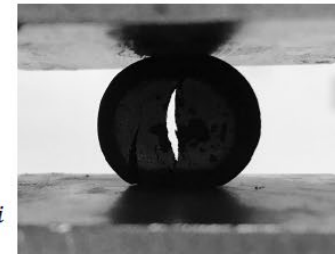
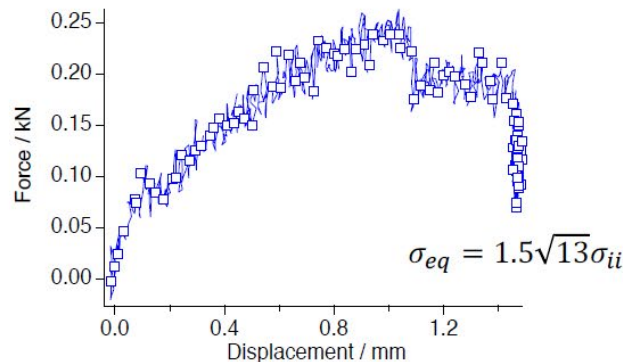
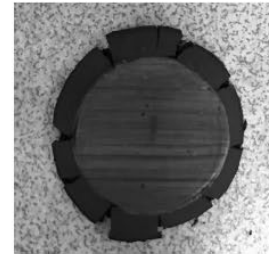
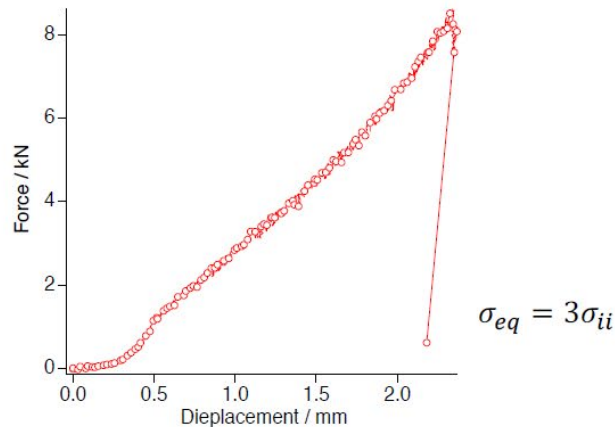
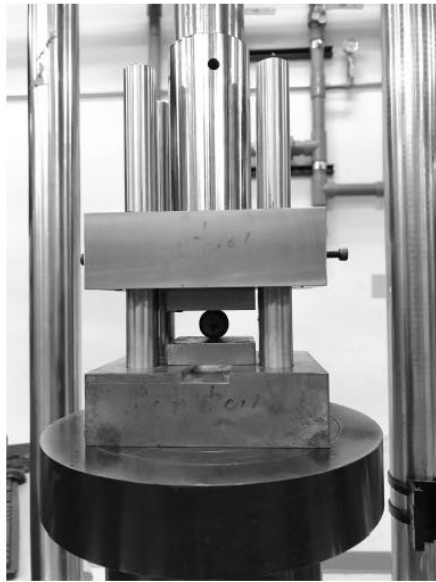
$$\theta = \frac{\tan \beta}{3\sqrt{3}} \quad \text{and} \quad \alpha = \frac{d}{\sqrt{3}}$$

- **The two material models used different expressions for limit parameters, but can be transferred between the two.**
- **MAT-145 is needed for cell simulation, but at this point we do not have parameters for its failure model.**
- **MAT-145 has many other parameters that will need to be estimated by experiments and simulations.**

Technical Progress: Material Model Development

Lateral and Axial Compression on Cathode Material

Axial compression and lateral compression of cathode material



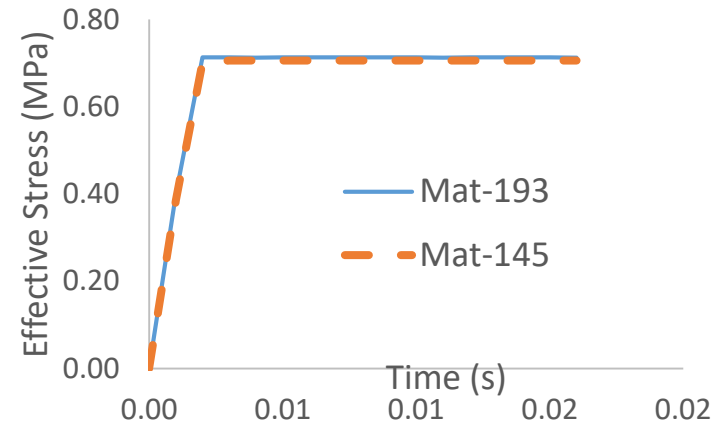
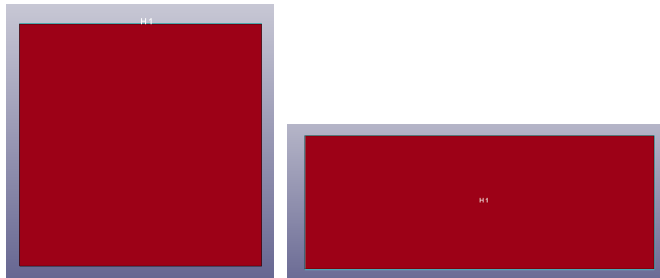
- There are no standardized tests for characterization of active materials.
- We are developing tests in other projects to develop the methods.
- In this case, axial and lateral compression give two points in the pressure, shear space that can be used to define limit surface for the Drucker-Prager model.

Technical Progress: Material Model Development

Simulations with Measured Material Properties_Anode

- One element test, uniaxial compression.
- Anode active material $C = 59.5$ kPa and $\phi = 70.9^\circ$.
- The two material models give same response which just confirms transfer of parameters between the formulations.

Compression, 1 element

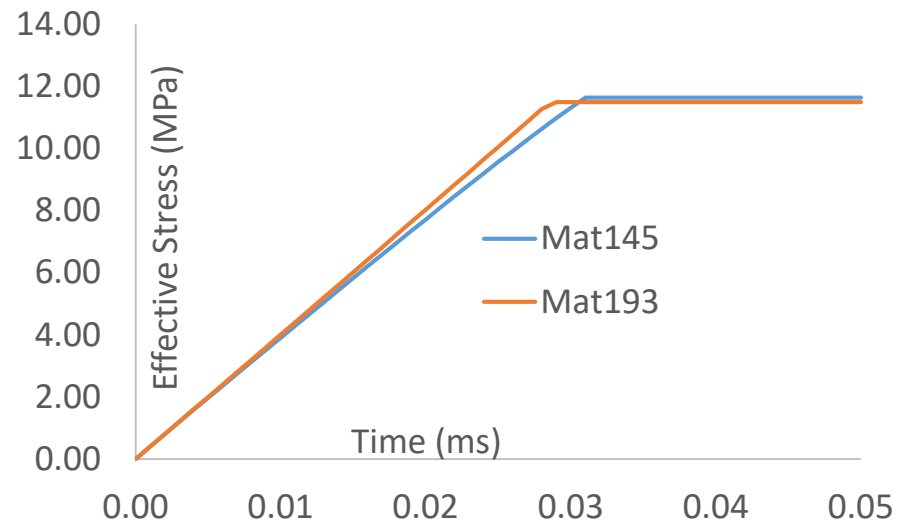
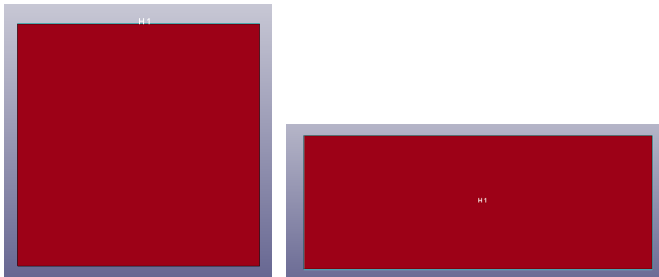


Technical Progress: Material Model Development

Simulations with Measured Material Properties_Cathode

- One element test, uniaxial compression.
- Cathode active material $C = 0.783$ MPa and $\phi = 74.8^\circ$.
- The two material models give same response which just confirms transfer of parameters between the formulations.

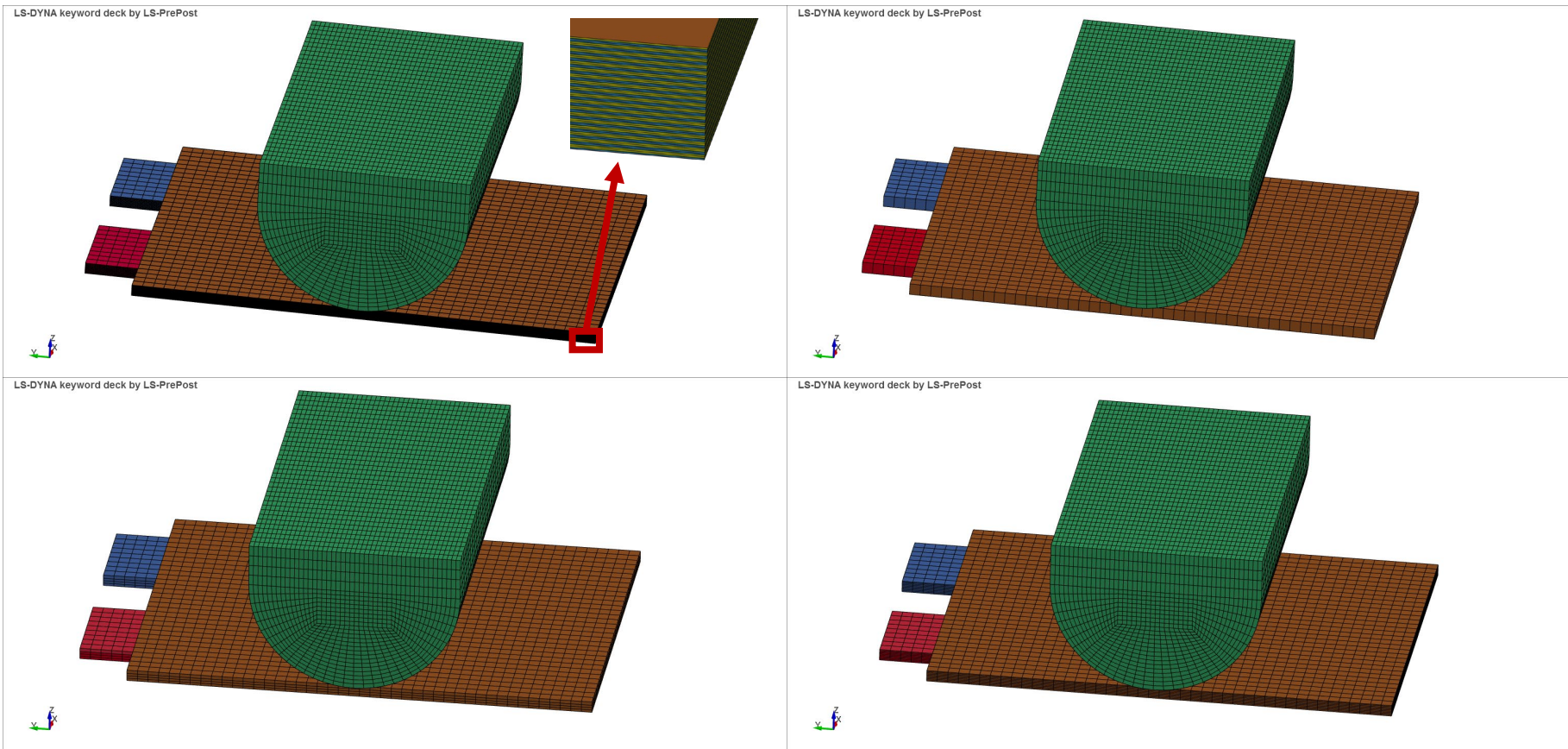
Compression 1 element



Technical Progress: LS-DYNA Solver Development

EM and Thermal Solver Development

- Note: ORNL uses the term 'layered solid element' while Ford uses 'composite t-shell element'. They are the same and can be used interchangeably.



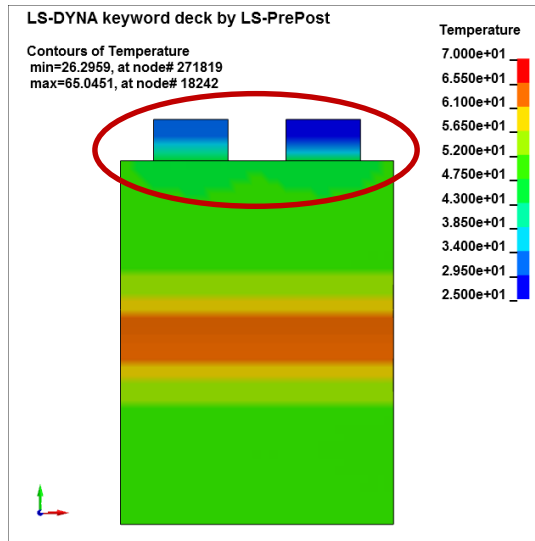
- Models with standard solid elements and composite tshell elements, where the number of tshell elements in the thickness direction is 1, 4 and 9.

Technical Progress: LS-DYNA Solver Development

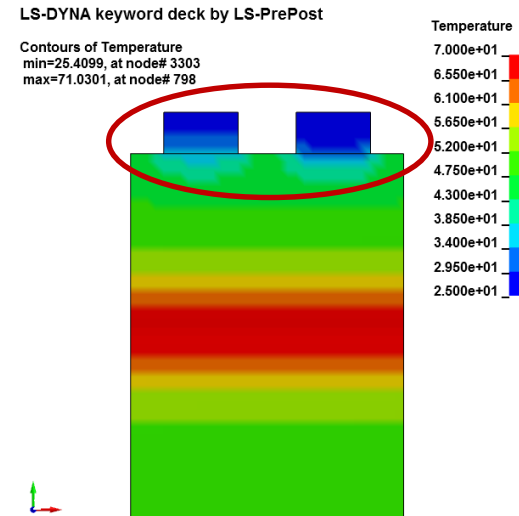
EM and Thermal Solver Development

- Temperature around cell terminals is slightly different in models.

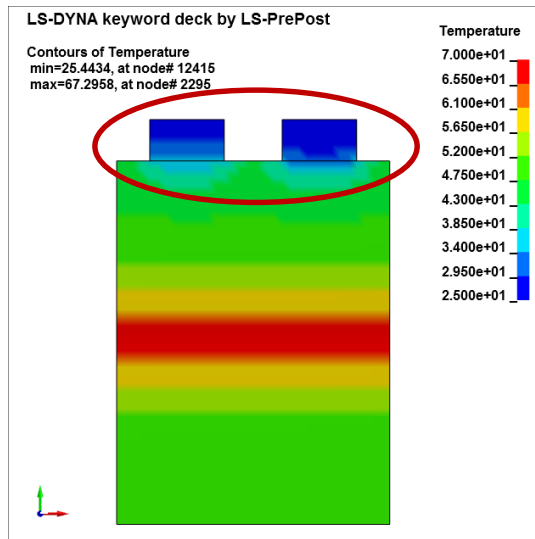
Solid



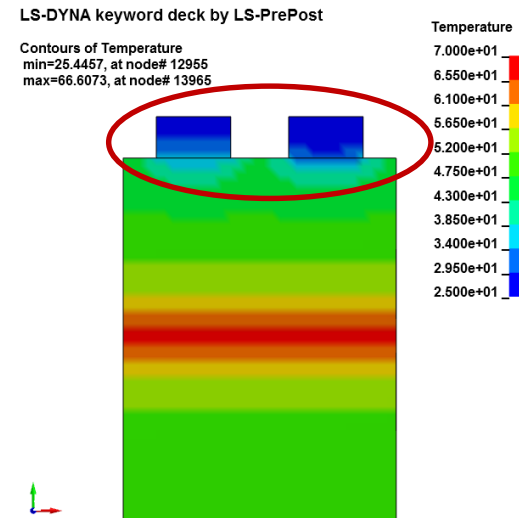
Tshell_1



Tshell_4



Tshell_9

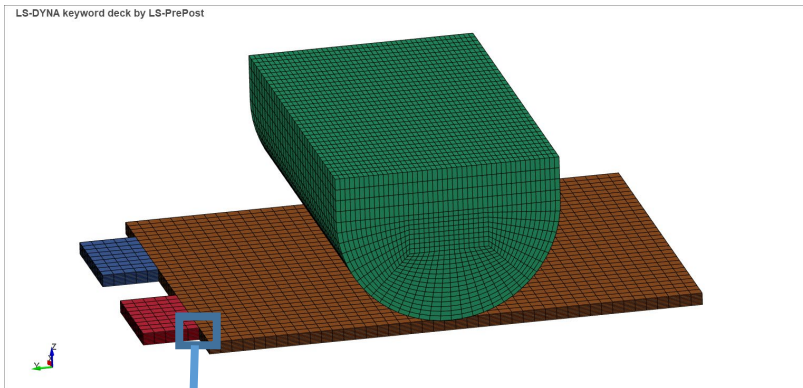


Technical Progress: LS-DYNA Solver Development

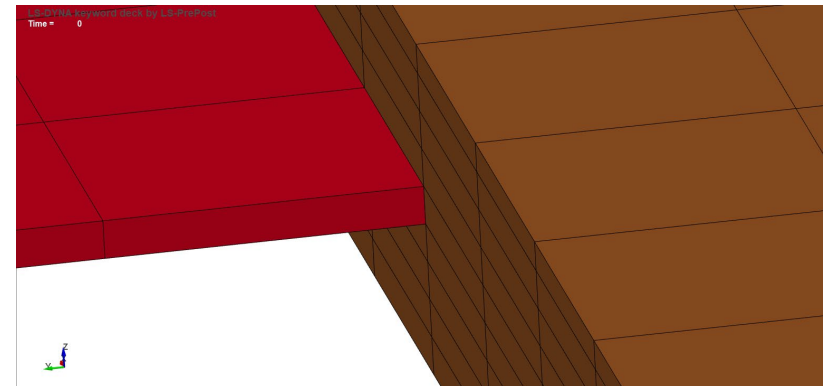
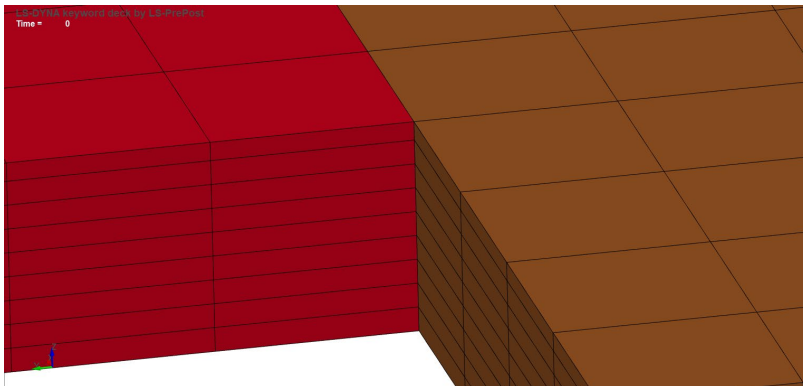
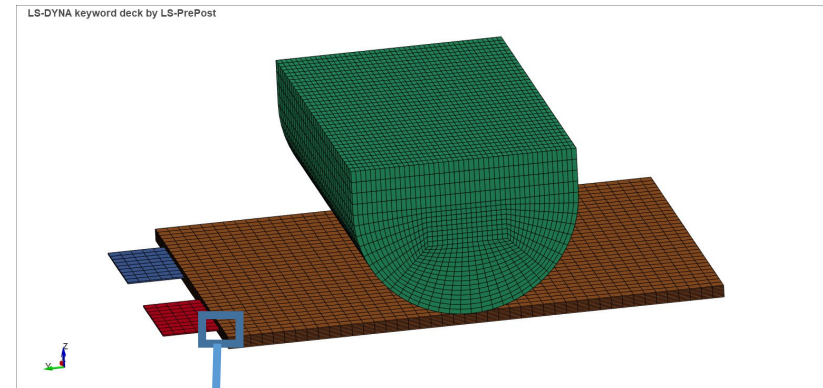
EM and Thermal Solver Development

- Improve the temperature prediction around cell terminals by reducing the number of elements in cell terminals.

Tshell_9



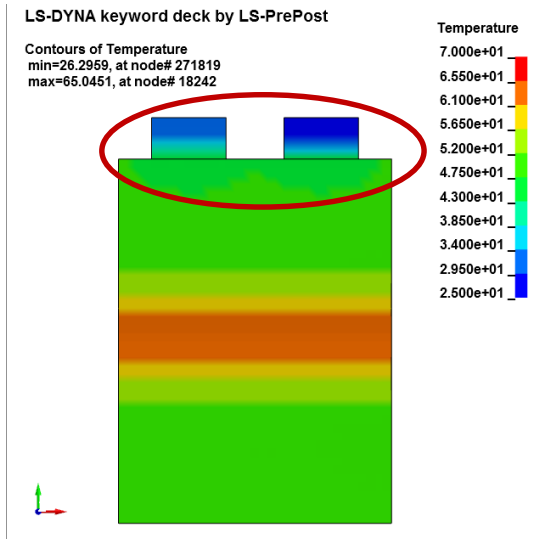
Tshell_9b



Technical Progress: LS-DYNA Solver Development

EM and Thermal Solver Development

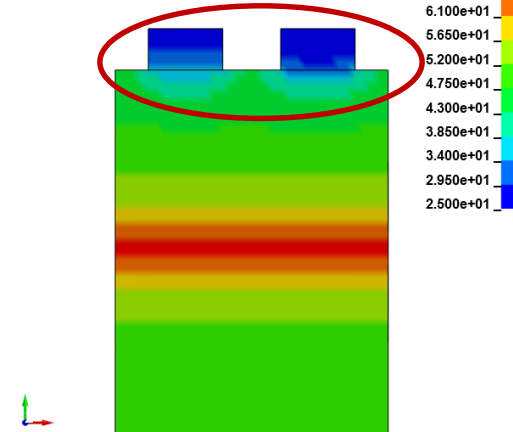
Solid



Tshell_9

LS-DYNA keyword deck by LS-PrePost

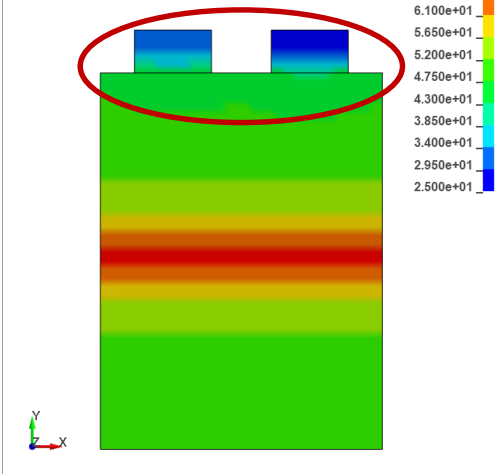
Contours of Temperature
min=25.4457, at node# 12955
max=66.6073, at node# 13965



Tshell_9b

LS-DYNA keyword deck by LS-PrePost

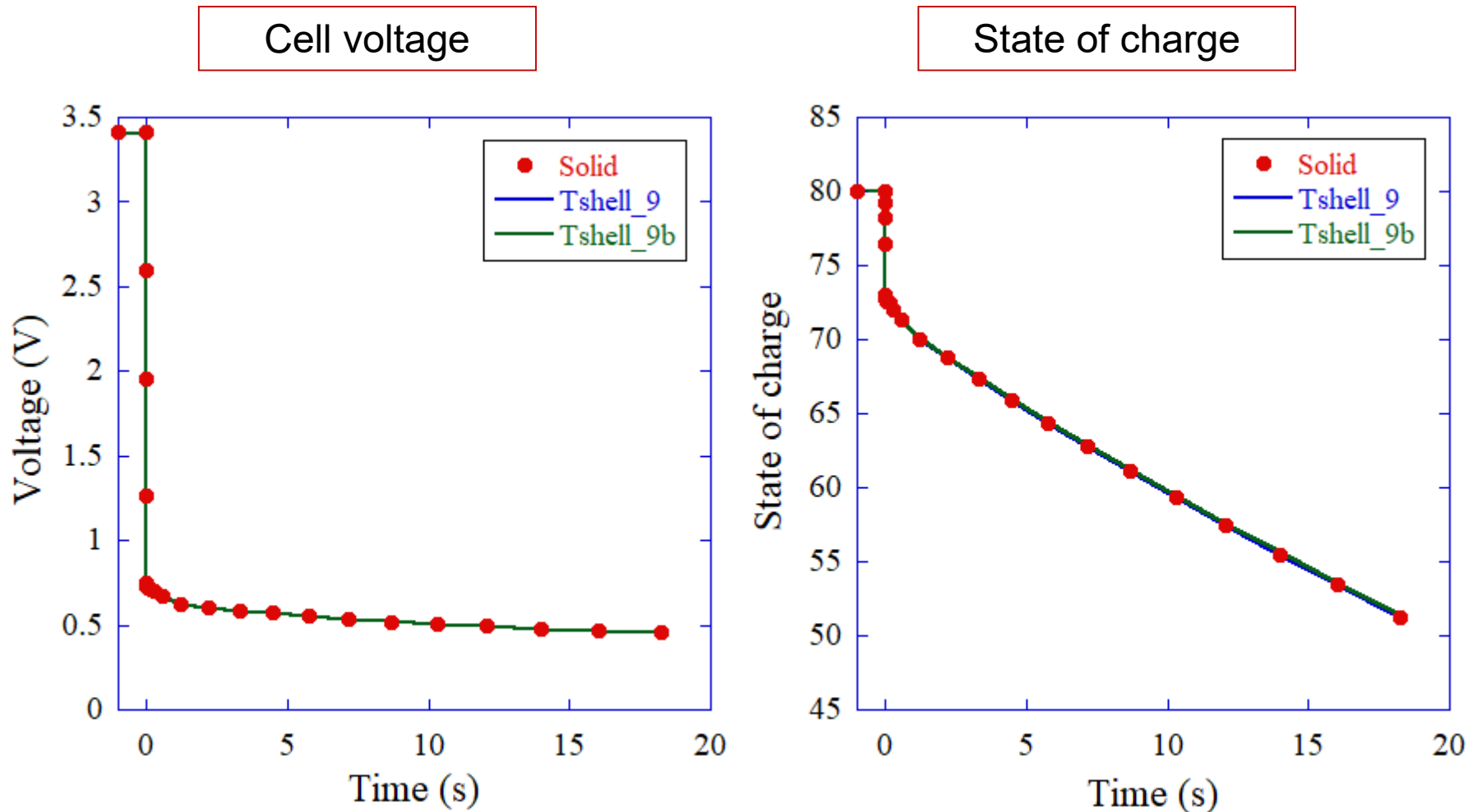
Contours of Temperature
min=26.0954, at node# 19615
max=66.6089, at node# 13972



Technical Progress: LS-DYNA Solver Development

EM and Thermal Solver Development

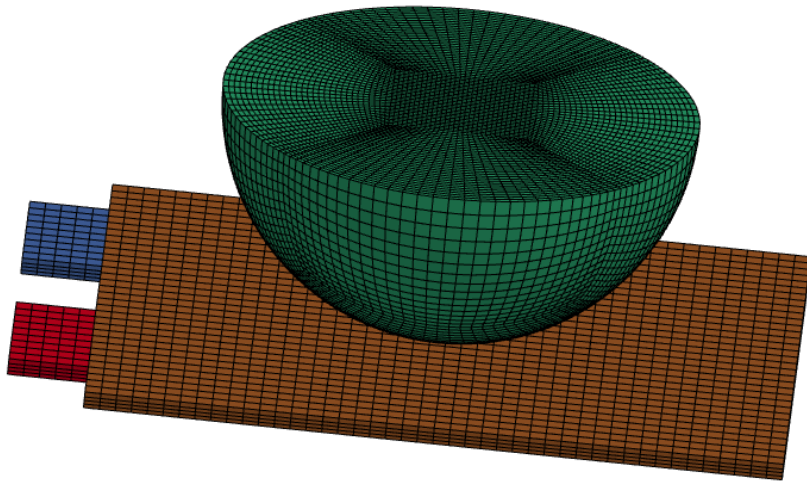
- Comparison of cell voltage and SOC evolution showing no simulation impact associated with reduction in cell terminal elements.



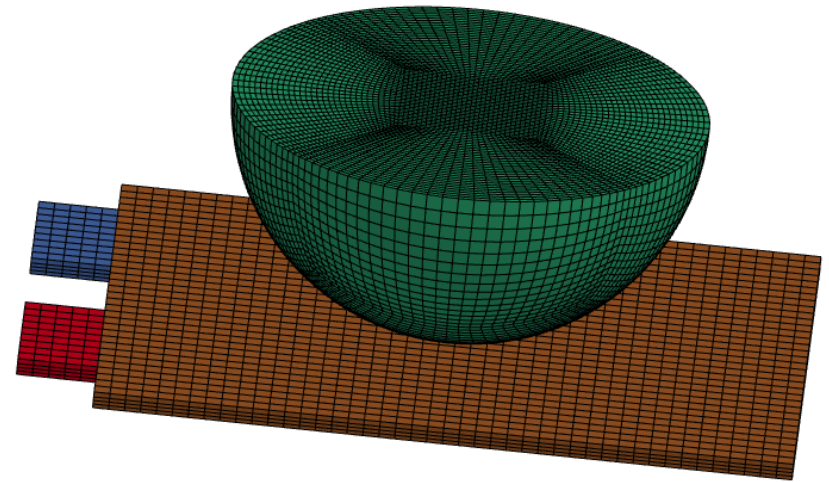
Technical Progress: LS-DYNA Solver Development

Macro Model Development

Composite tshell model



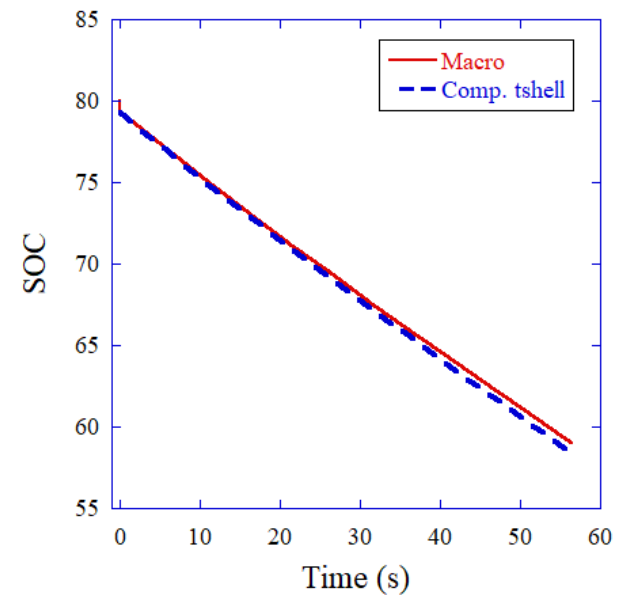
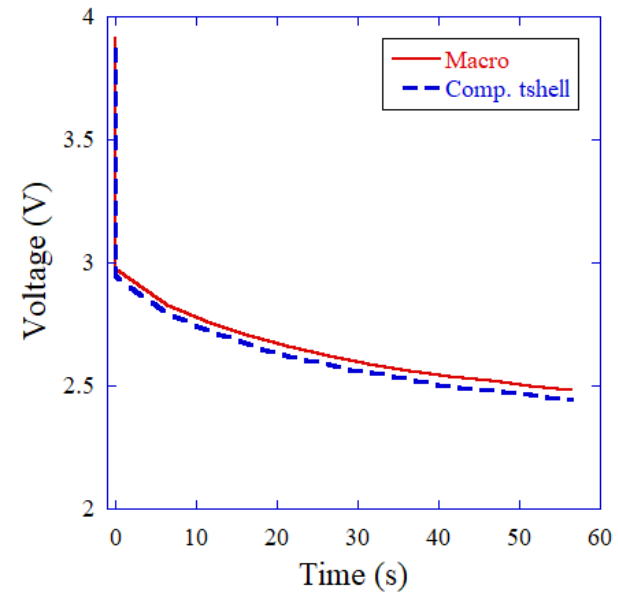
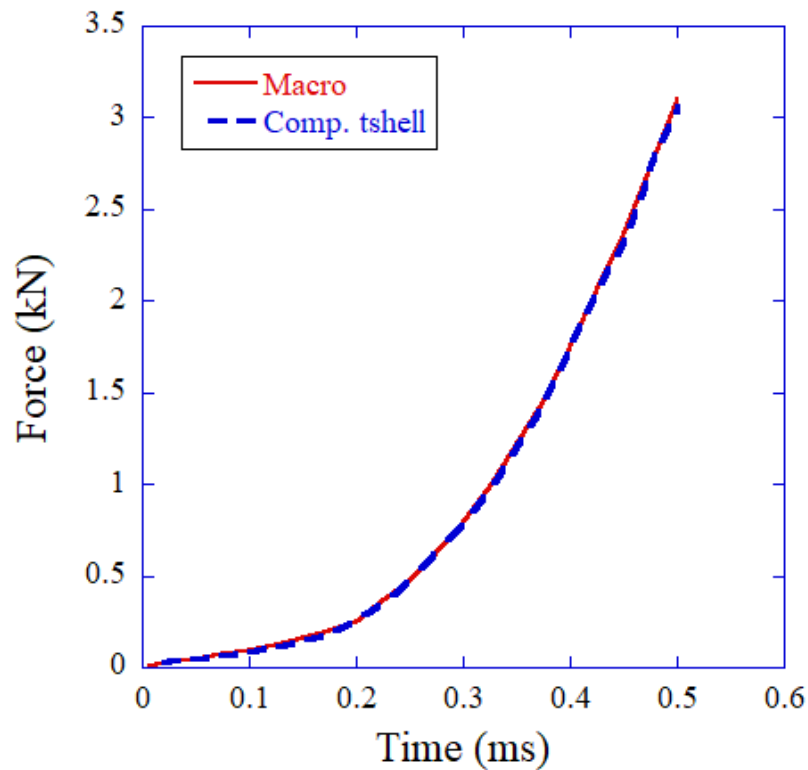
Macro model



- Both models have the same mesh, material properties and boundary conditions.
- In the composite tshell model, each element contains multiple integration points that correspond to individual layers. Solid elements are used in the macro model.
- Short-circuit conditions are different in two models.

Technical Progress: Macro Model Development

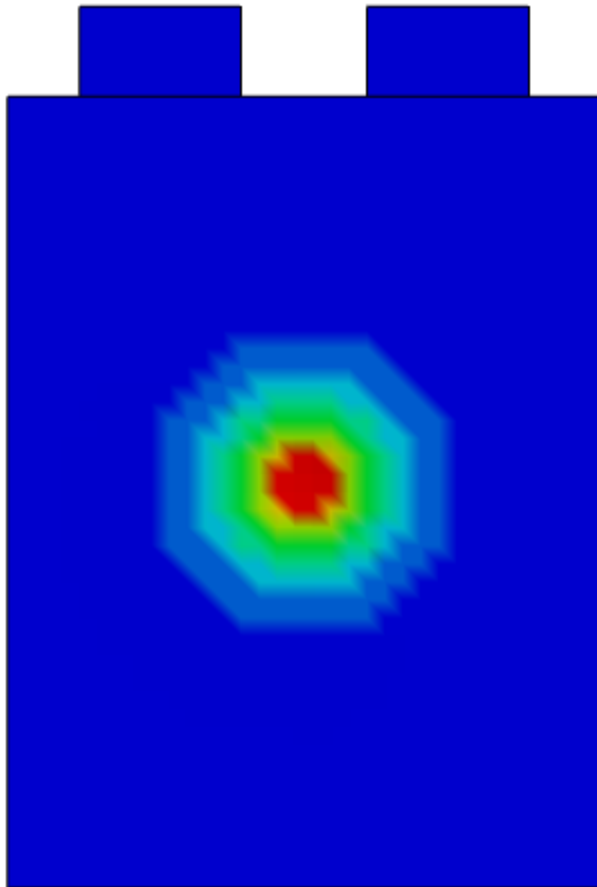
Model Comparison_Macro vs Composite t-Shell



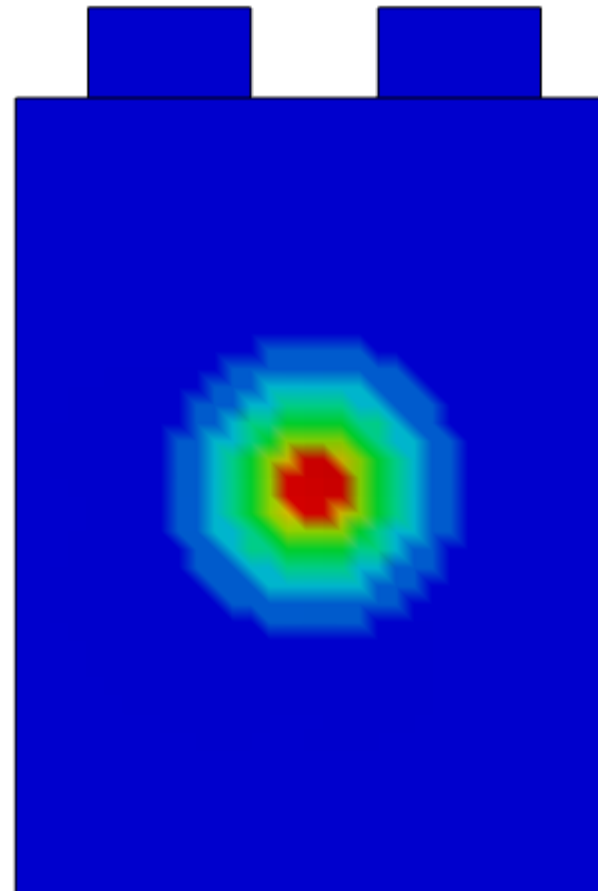
Technical Progress: Macro Model Development

Model Comparison_Macro vs Composite t-Shell

Composite tshell model



Macro model



Temperature

1.600e+02

1.465e+02

1.330e+02

1.195e+02

1.060e+02

9.250e+01

7.900e+01

6.550e+01

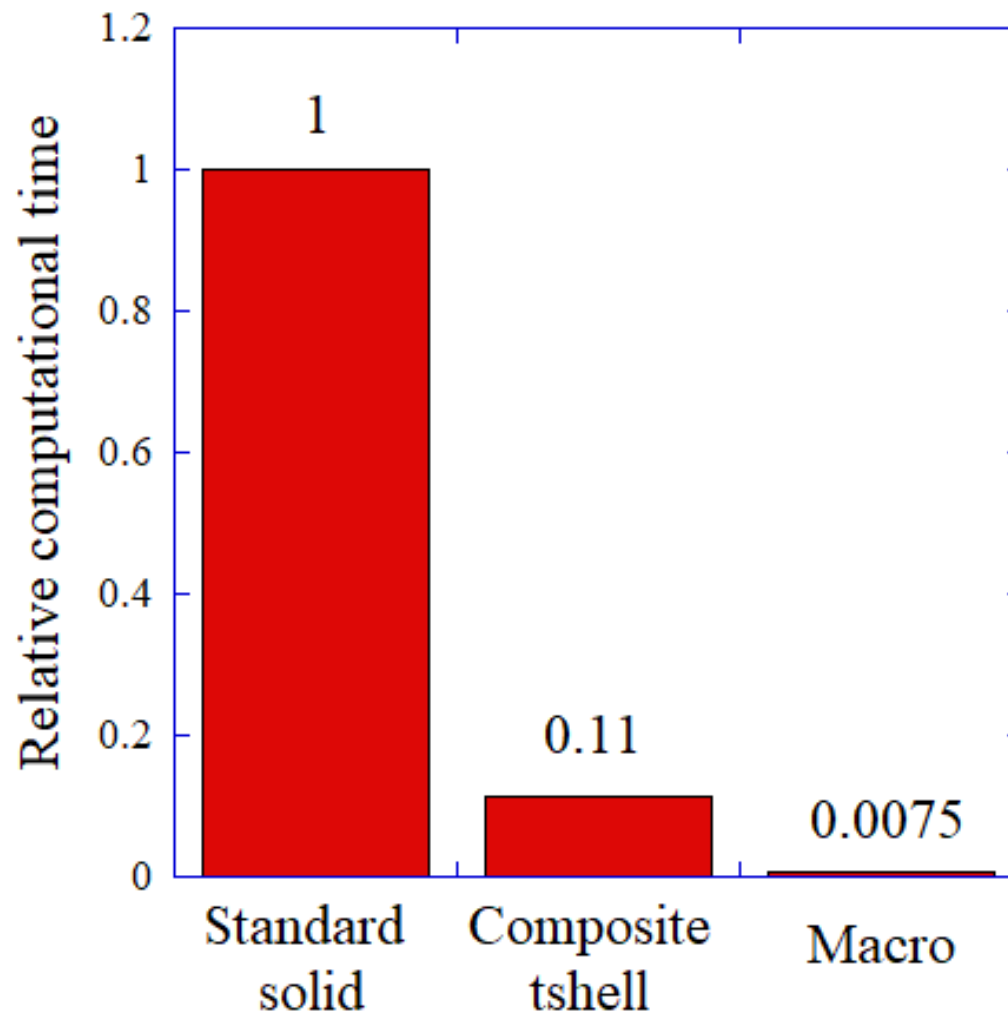
5.200e+01

3.850e+01

2.500e+01

Technical Progress: Macro Model Development

Comparison of Computational Time



Responses to Previous Reviewers' Comments

- **Comment**

- In the development of the layered solid solver, the anodes and cathodes are represented by the same model, MAT-63. However, the physical and electrochemical properties for the anode and cathode may vary a lot. The reviewer asked if it is possible to develop different models for different materials.

- **Response**

- X-ray tomography of pouch cells that were exposed to different extent of lateral loading (shear, indentation) have shown that the active material layers in automotive Li-Ion batteries perform very similarly to granular materials with internal cohesion. This has also been indicated with recent papers (e.g. preprint https://www.researchgate.net/publication/331517820_Deformation_and_failure_of_lithium-ion_batteries_treated_as_a_discrete_layered_structure) and experiments conducted on active materials both in literature and in this project. Therefore, a practical approach for this class of battery cells is to select a type of material model (e.g. soils, concrete, asphalt) adequate for this class of active materials and use experiments to calibrate the values of the model parameters. The layered solid formulation also allows for placement of different types of material models and properties in different layers, so our layered solid models include elasto-plastic material models (e.g. MAT-24) for current collectors and separator, and pressure sensitive models (e.g. MAT-63, cap models, Drucker-Prager) for active materials.

Responses to Previous Reviewers' Comments Cont'd

- **Comment**

- In Slide 21, the reviewer could not find a clear difference between the standard and layered solid elements and asked for a detailed explanation.

- **Response**

- For layered solid elements, the EM and thermal solvers automatically build an internal mesh that is exactly the same as that in the standard solid element model. All equations are solved on the internal mesh in the EM and thermal solvers, so the standard and layered solid element models should have the same results in EM and thermal solver, and that is why the differences between two models is small in slide 21. Two models are not exactly the same in slide 21 because the thickness of elements in cell terminals are different.

Collaborations and Coordination



- ORNL is developing methods to scale-up detailed mechanical simulation to reduce computational complexity while retaining high fidelity.



- LS-DYNA® is the CAE software of choice for the project and contains key, battery-specific solver enhancements.



- South West Research Institute has designed the prototype tests stands and is running model validation tests. SwRI also runs X-CT analyses to better understand the failure mechanisms during tests for the development of failure models.

Remaining Challenges and Barriers/ Future Research

- **Remaining Challenges and Barriers**

- Ford team found test quality issues from the previous testing company. Also, high speed impact testing is behind the original schedule due to lack of sophisticated equipment and resources at the previous test supplier company.
- For the successful delivery of the failure model(s), extensive analysis of the deformed cells is required to better define the failure mechanisms.

- **Future Research**

- New test company (SwRI) was selected and completed the test stand build up. Initial tests were carried out to make sure all test equipment worked as expected and all of the required data could be obtained from the tests. All of the high speed impact and quasi-static tests (rerun) will be completed in early 2Q, 2019.
- New material models for active material layers will be developed using parameters extracted from tests done in this year and will be validated with the layered solid elements solver.
- Additional crush tests are designed and will be carried out with 0% SOC cells for non-destructive analysis of the deformed cells to define the deformation mechanisms of the cell during the high speed impact tests and associated cell failure mechanisms.
- By expanding the project scope, ORNL and LSTC teams will work together for the development of the failure models with which simulation can continue after the onset of failure.

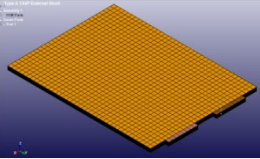
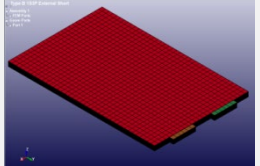
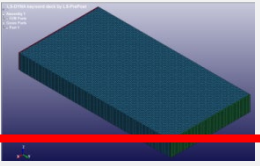
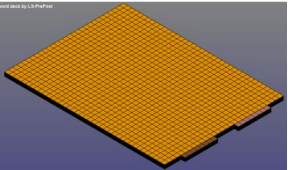
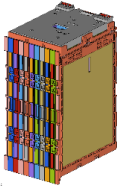
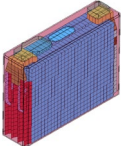
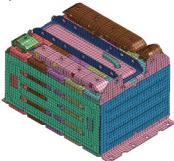
Summary

- Through the technical due-diligence, SwRI was selected to conduct the high speed impact tests and rerun the quasi-static tests. SwRI completed test setup and preliminary tests proving their capability of rigorous testing. The expected testing will be completed in the next few months.
- The use of composite t-shell elements (= layered solid elements) in mechanical, electromagnetic and thermal solvers has been demonstrated to greatly reduce computational time while maintaining accuracy.
- Development of the macro model was initiated aiming to improve computational efficiency of the EM and thermal solvers.
- By using X-ray computed tomography, damage in individual cell layers under shear and compression was investigated.
- New material models were being developed to treat active materials as granular materials with parameters chosen to yield good results compared to experiments.

Technical Backup Slides

Hardware Selection

Type D and Type E modules were selected in 2017 for β -model development

Mesh/Geometry	Type	Cathode Chemistry and Format	Cell	Module	Pack
	A	NMC//LMO Blend Pouch	15 Ah 3.7 V 0.06 kWh	4P1S 5P4S	4S5P (x9) + 2S5P (x2)
	B	NMC Pouch	20 Ah 3.6 V 0.07 kWh	3P1S and 3P10S	
	C	LFP Prismatic	18 Ah 3.2 V 0.06 kWh	4P1S 5P2S	36S5P
	D	NMC Pouch	21 Ah 3.65 V		4S5P (x9) + 2S5P (x2)
	E	Metal Oxide Blend Prismatic	63 Ah 3.65 V (est)		1P5S (X11) + 1P6S (X7)

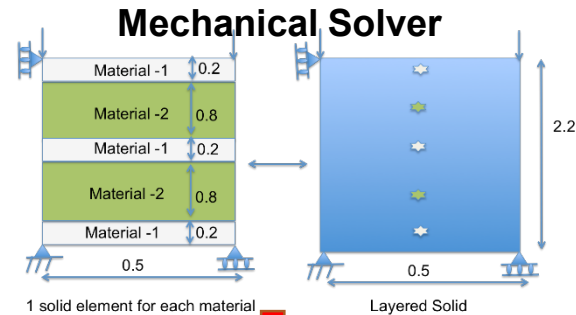
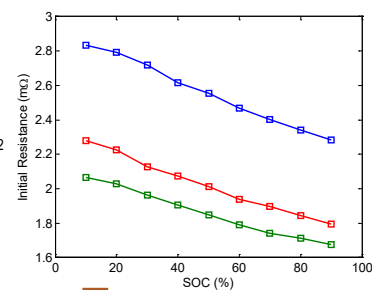
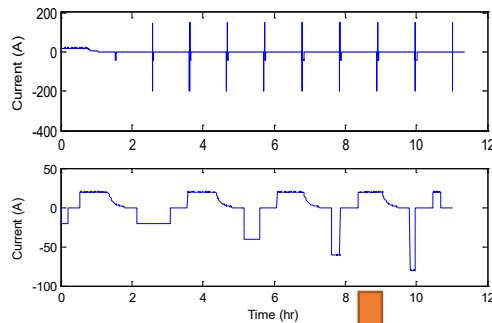
Legacy Hardware



Hardware sourced for this project

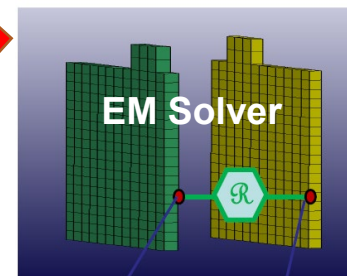
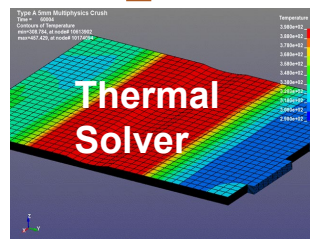
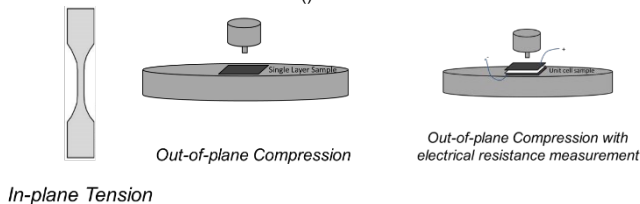
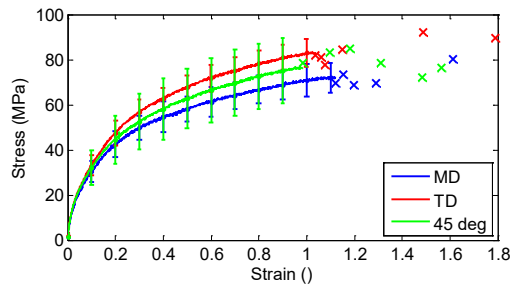
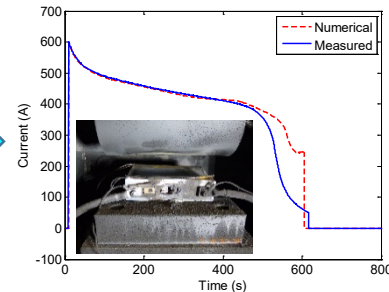


Approach – α Version Model Development Overview

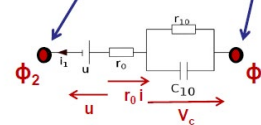


**Mechanical,
Electrochemical, and
Thermal Models**

**Solvers for PDEs
[Solid Element (α) \rightarrow Layered
Solid Element formulation (β)]**



Model calibration



**Model validation tests and
comparison of simulation
data vs. empirical data**

Approach – β Version Model Development Overview

